AGENTFATE

Evaporation of Chemical Warfare Agent HD on Glass Surface Under Various Environmental Conditions

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15 November 2004

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **15 NOV 2004**	2. REPORT TYPE **N/A**	3. DATES COVERED **-**

4. TITLE AND SUBTITLE **Evaporation of Chemical Warfare Agent HD on Glass Surface Under Various Environmental Conditions**	5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **U.S. Army Edgewood Chemical Biological Center, APG, MD**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S) 11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001849, 2004 Scientific Conference on Chemical and Biological Defense Research. Held in Hunt Valley, Maryland on 15-17 November 2004 . , The original document contains color images.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**UU**	**50**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

ABSTRACT

Environmental fate of the chemical warfare agents (CWA) is receiving increasing attention, since the evaluation of the contact or vapor hazard is the critical input for models employed to support decisions to determine the individual as well as collective protection level of the combatants. Once released, CWA might evaporate and be carried by the wind, sorb into the surface material, or both. This can be a function of not only CWA, its dropsize and the surface substrate but also the environmental factors such as temperature, relative humidity, and wind speed. This work was carried out to establish a better understanding of the influence of each factor to the fate of CWA. Two different microbalances, configured in a wind-tunnel geometry, were employed to measure the weight loss of HD as a function of time from glass surface under various environmental conditions.

Instrumentation for Microbalance Wind Tunnel

- Dual beam, horizontal microbalance with simultaneous differential thermal analysis (TA Model SDT-Q600)
- Evolved gas geometry, vertical microbalance (TA Model TGA-2950)

Figure 1. TA Vertical Microbalance with Evolved Gas Option Allowing Use as an Horizontal Wind Tunnel

Figure 2. Horizontal Wind Tunnel Mode of the TA Model 2950 Microbalance

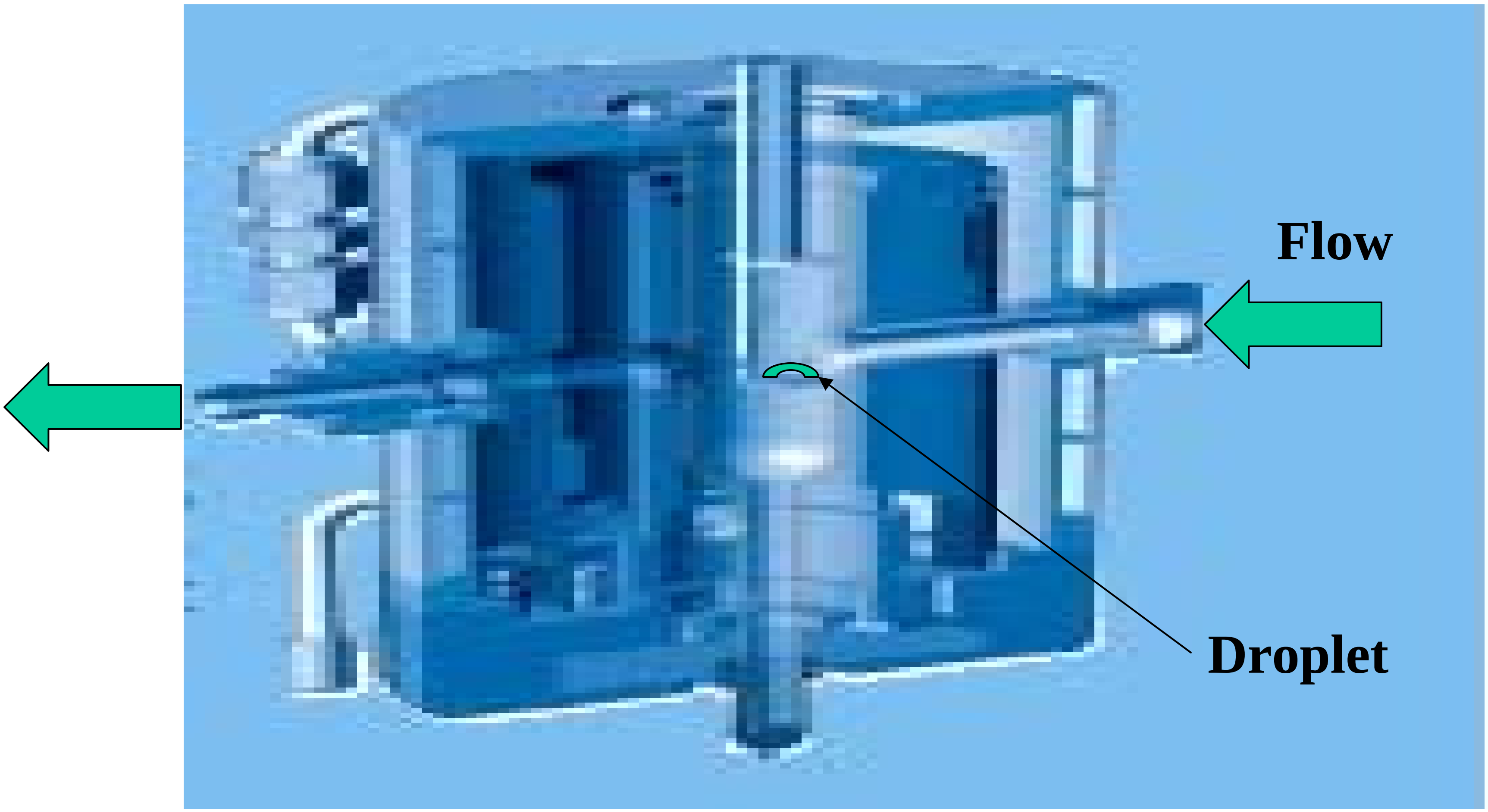


Figure 3. Sample/Control Thermocouple: TA Model 2950

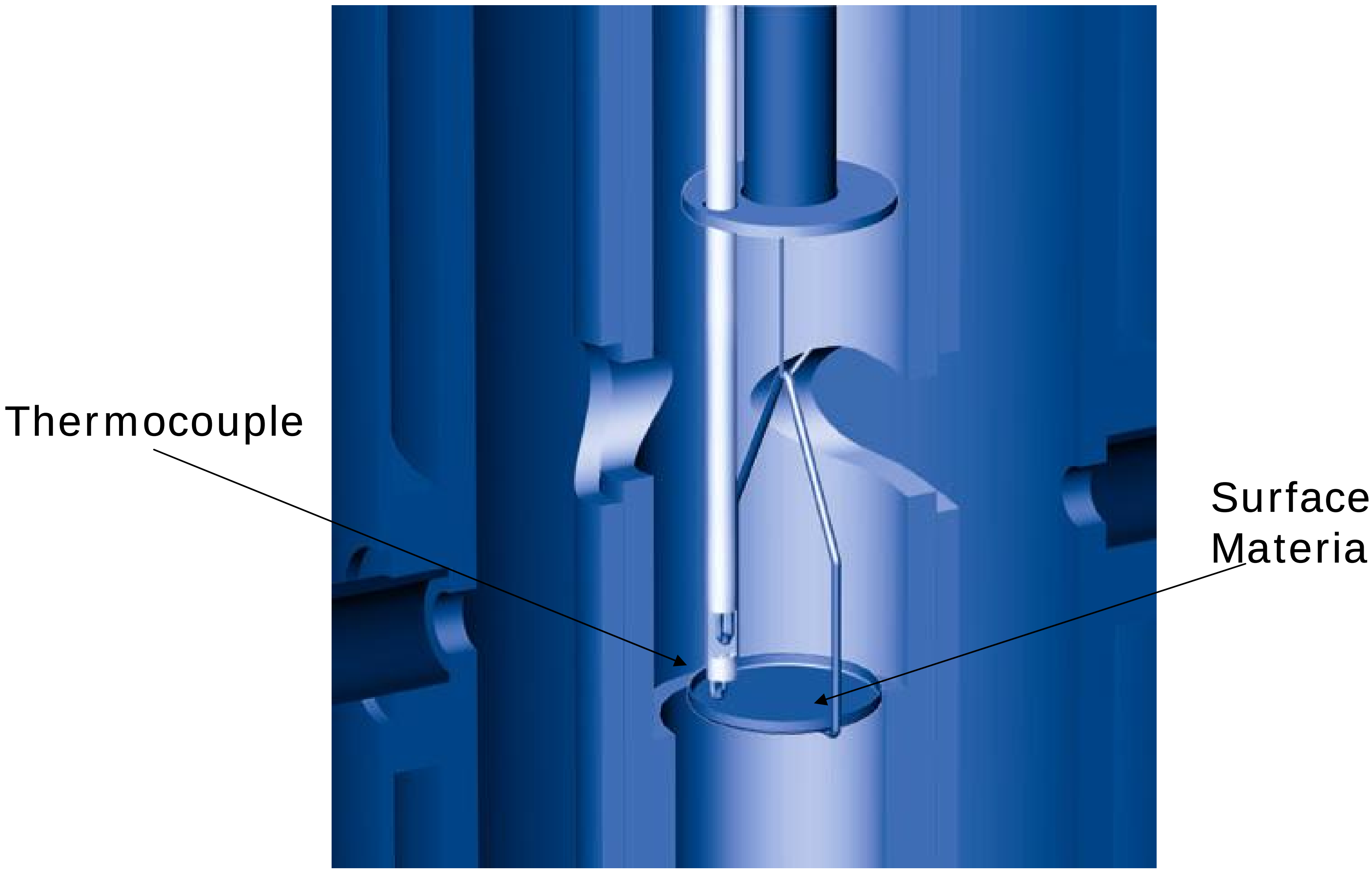


Figure 4. Q600 Simultaneous DSC-TGA

Figure 5. Horizontal Microbalance TA Q600 Showing Sample and Reference Holder

Q600 Reactive Gas Tubing

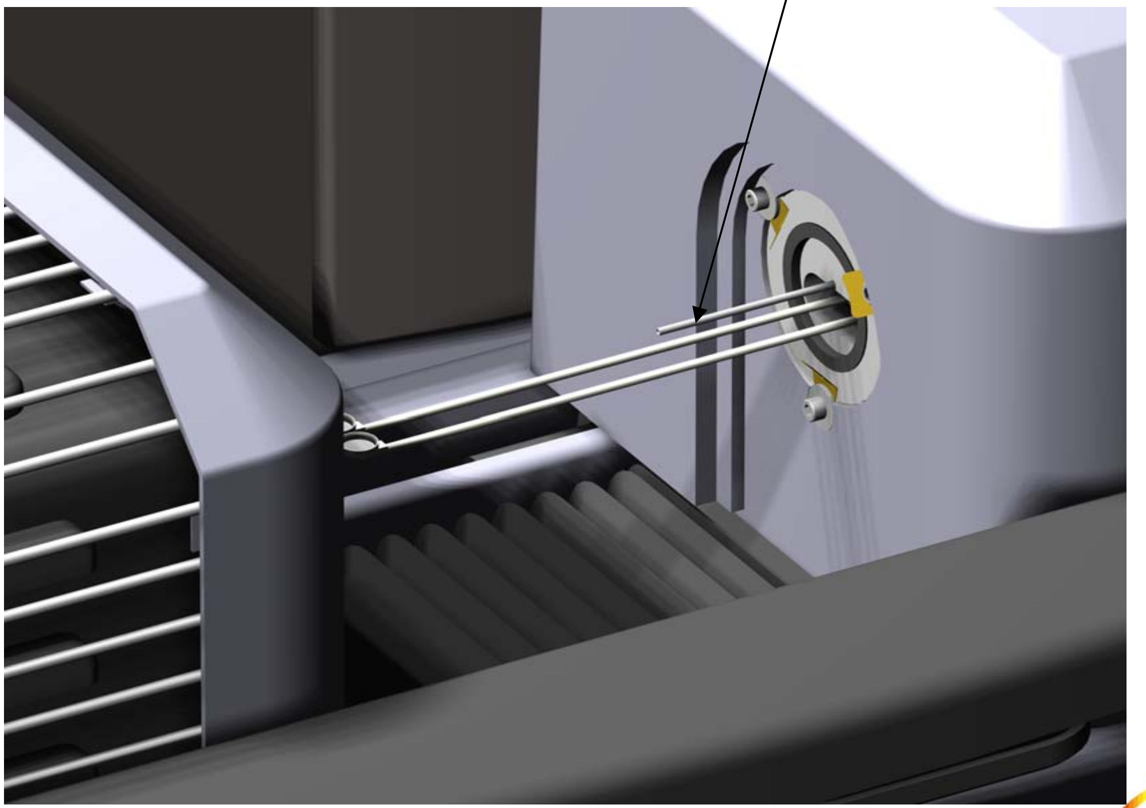
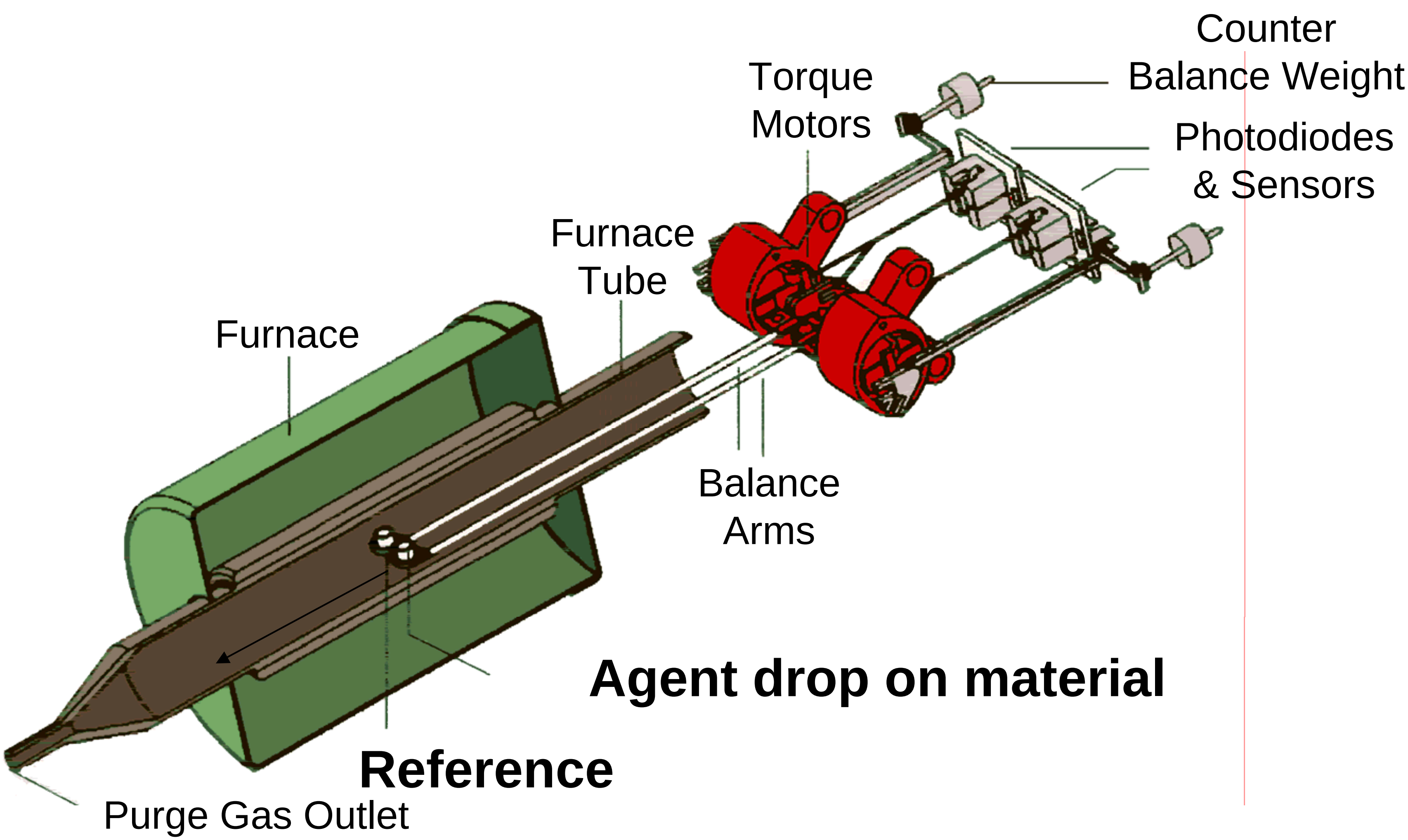


Figure 6. TA Model Q600



Surface Material

- COVER GLASS
  - 5mm (UNCLEANED AND CLEANED)
- WINDOW GLASS
  - 9mm for 2950 and 6mm for Q600 (CLEANED)
- TNO GLASS
  - 9mm for 2950 and 6mm for Q600 (CLEANED)
- Aluminum
  - Unpainted Floor of Aluminum 2024 on C17 Cargo Aircraft (from Tim Provens, WPAFB)
- Aggregate
  - Alabama Limestone

Experimental

- Temp: 25, 30, 40, and 55 C.
- Relative Humidity: 0 – 50%
- Drop Size: 0.91, 3.5 and 6 uL
- Flow Rate: 100, 500 and 1000 mL/min
- Purity of HD were 97+ % by GC/TCD.

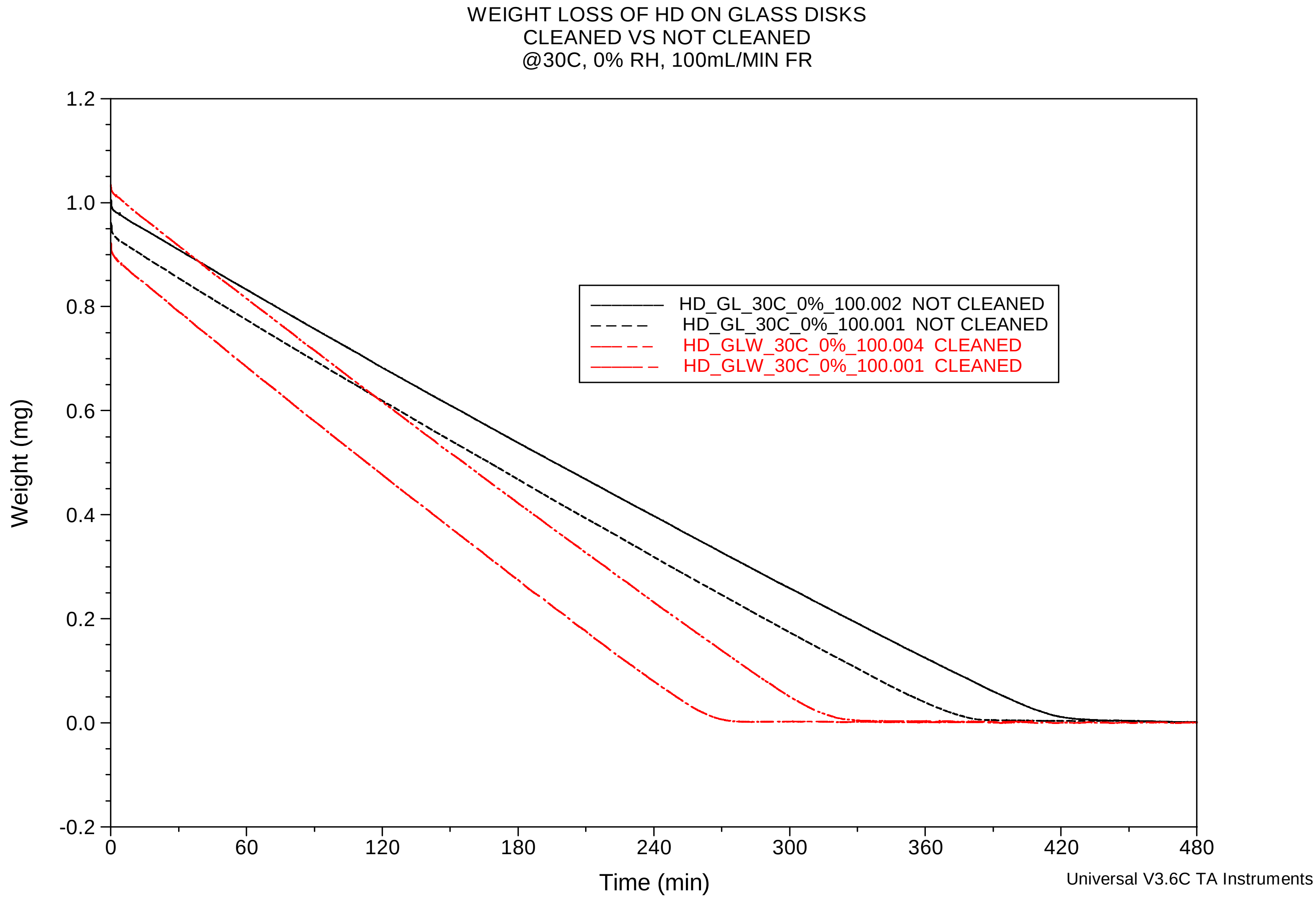


Figure 7. Comparison of HD Evaporation Rate from Glass (Cover)

Cleaned vs Uncleaned

@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate

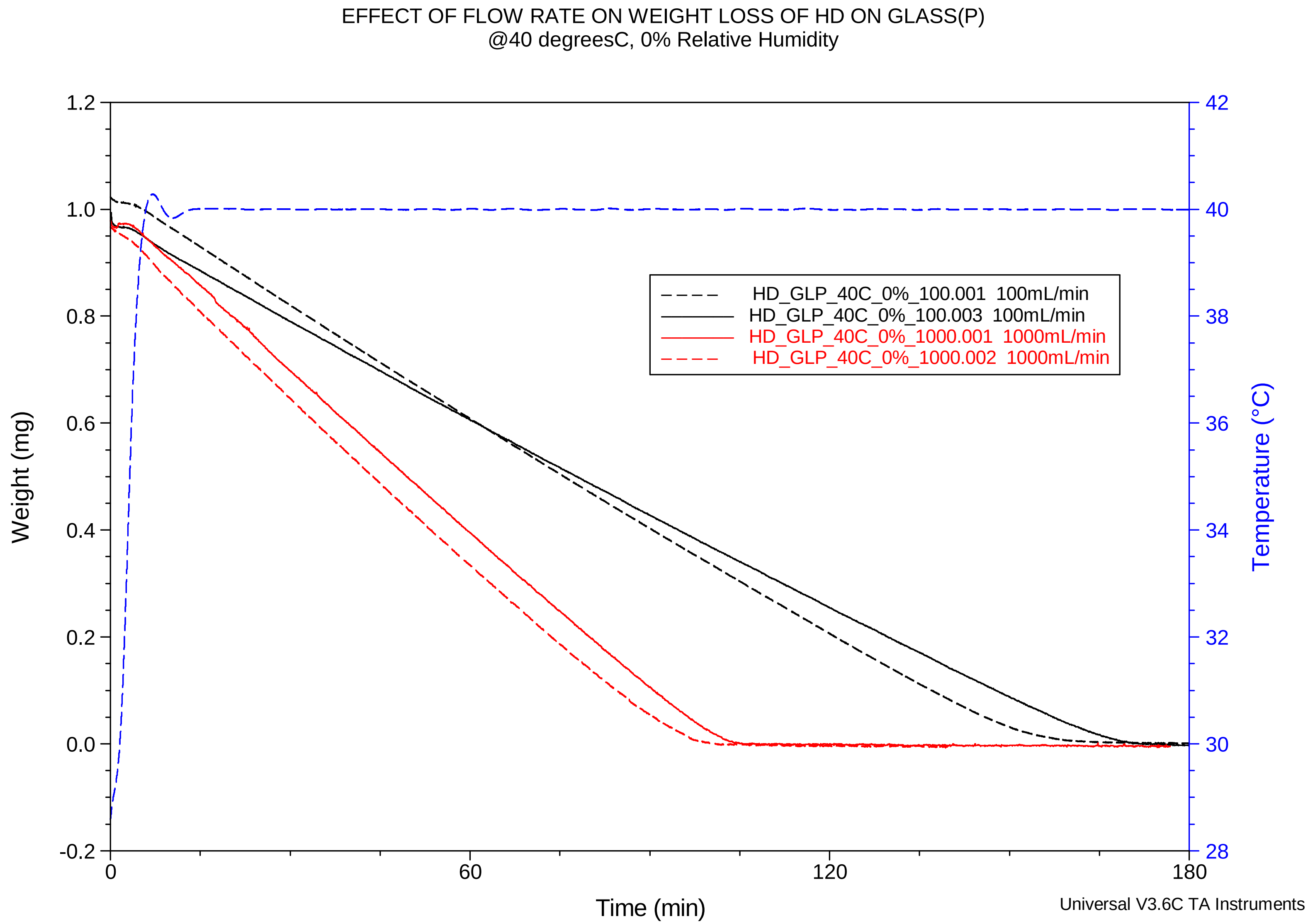


Figure 8. Comparison of HD Evaporation Rate from Glass (Window) at Various Flow Rates:
@40 degrees C, 0% Relative Humidity

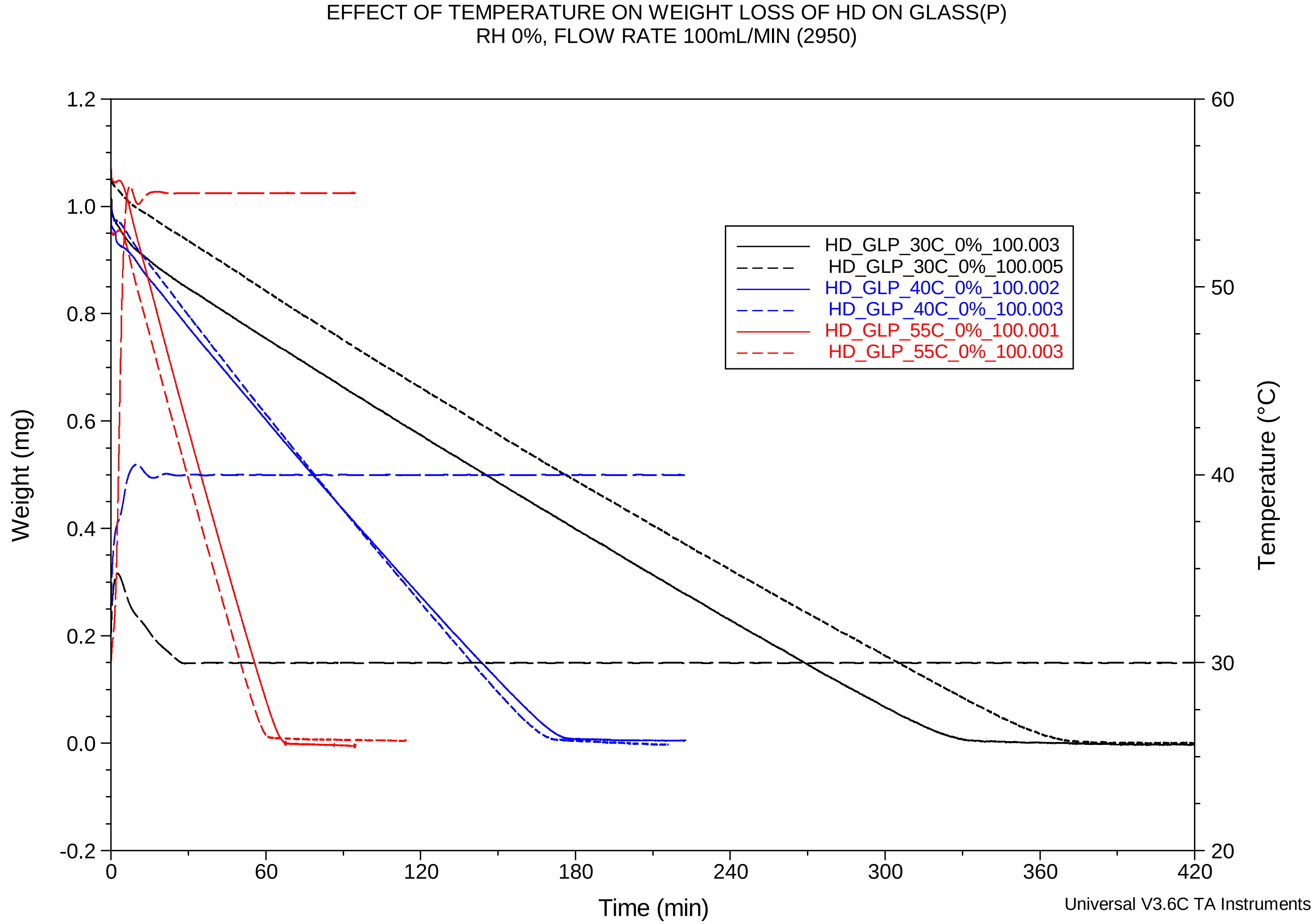


Figure 9. Comparison of HD Evaporation Rate from Glass(Window) at Various Temperatures: 0% Relative Humidity, 100 mL/min Flow Rate

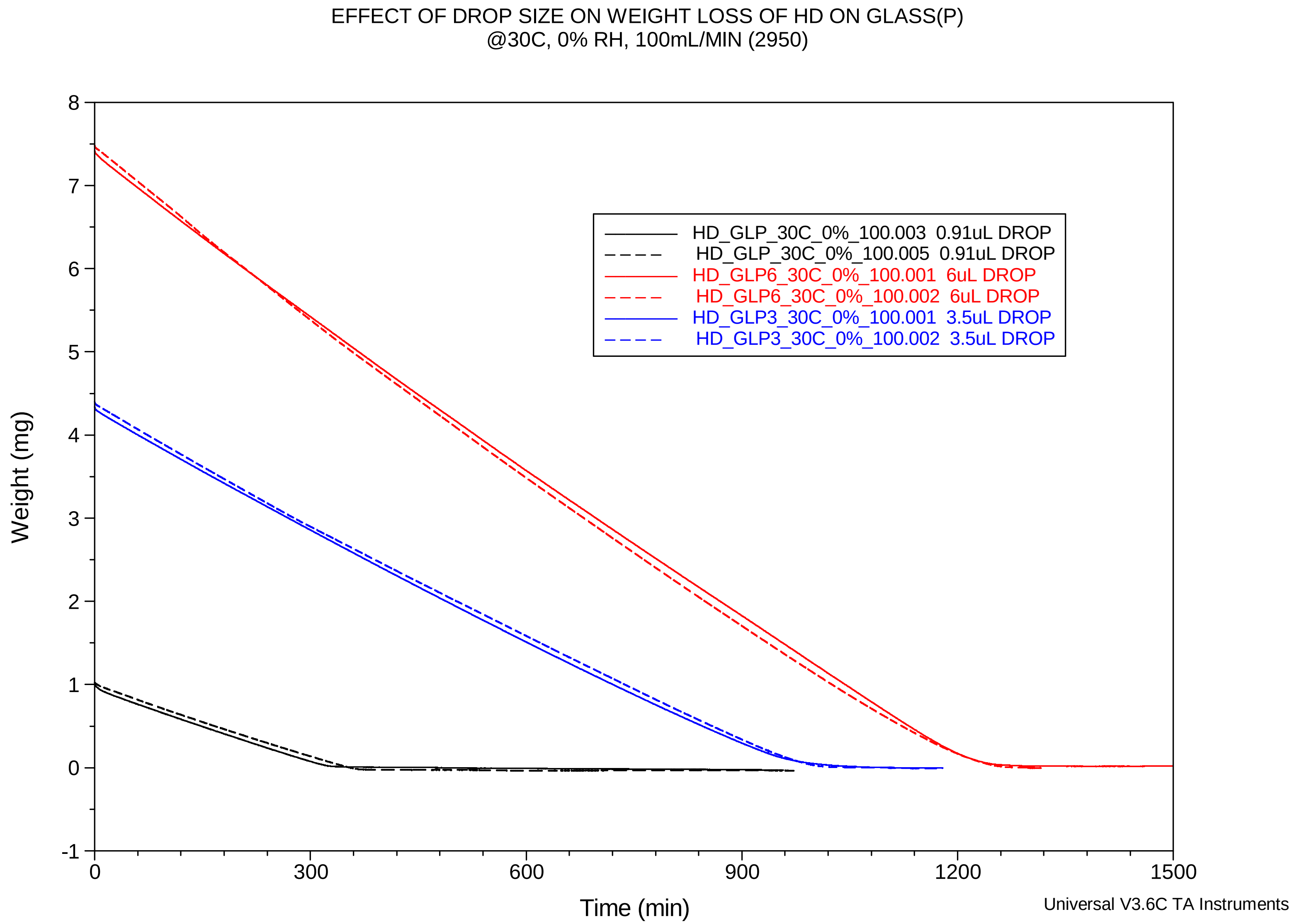


Figure 10. Comparison of HD Evaporation Rate from Glass (Window) from Various Drop Sizes:
@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate

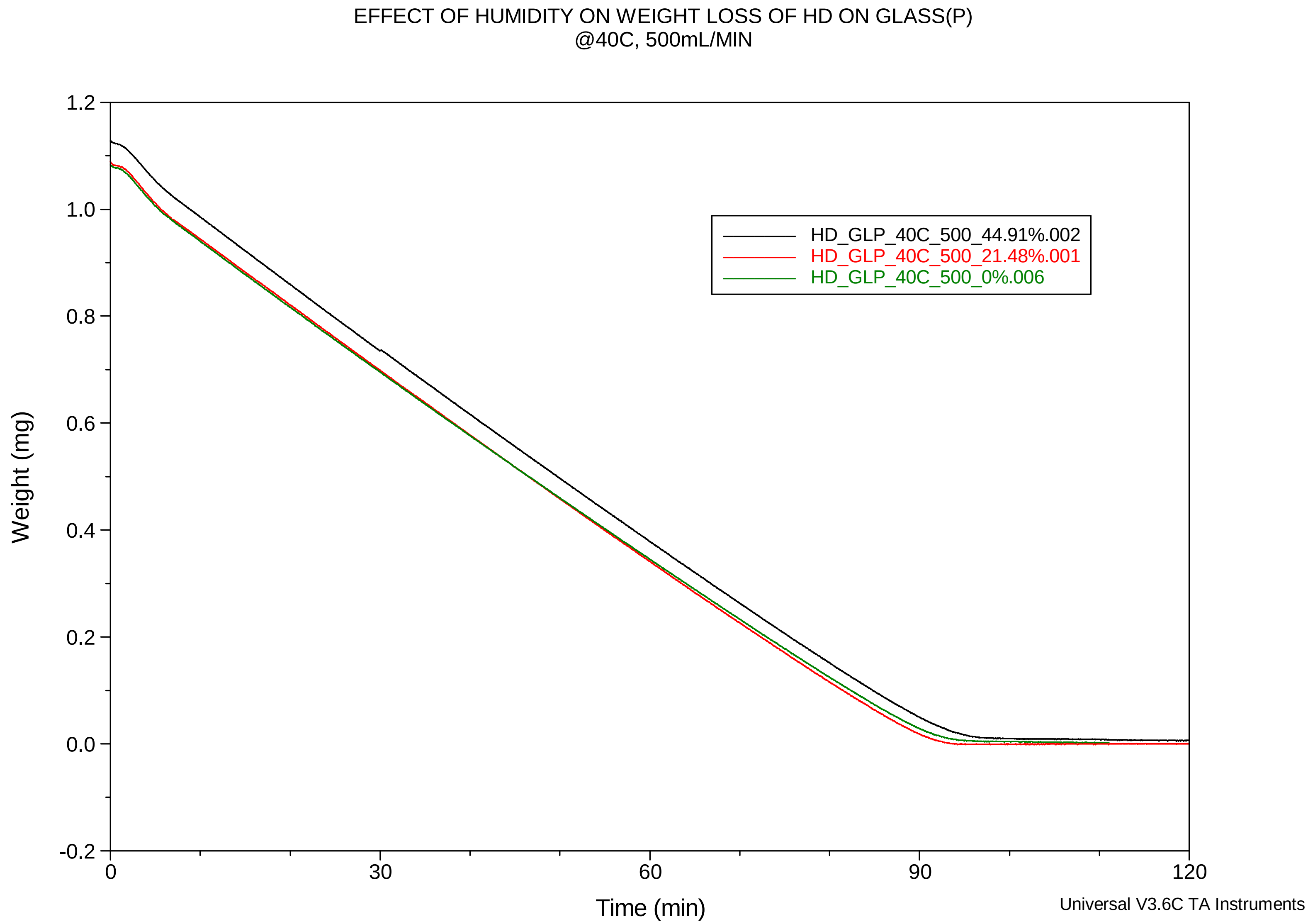


Figure 11. Comparison of HD Evaporation Rate from Glass (Window)
at Various Relative Humidities:
@40 degrees C, 500 mL/min Flow Rate

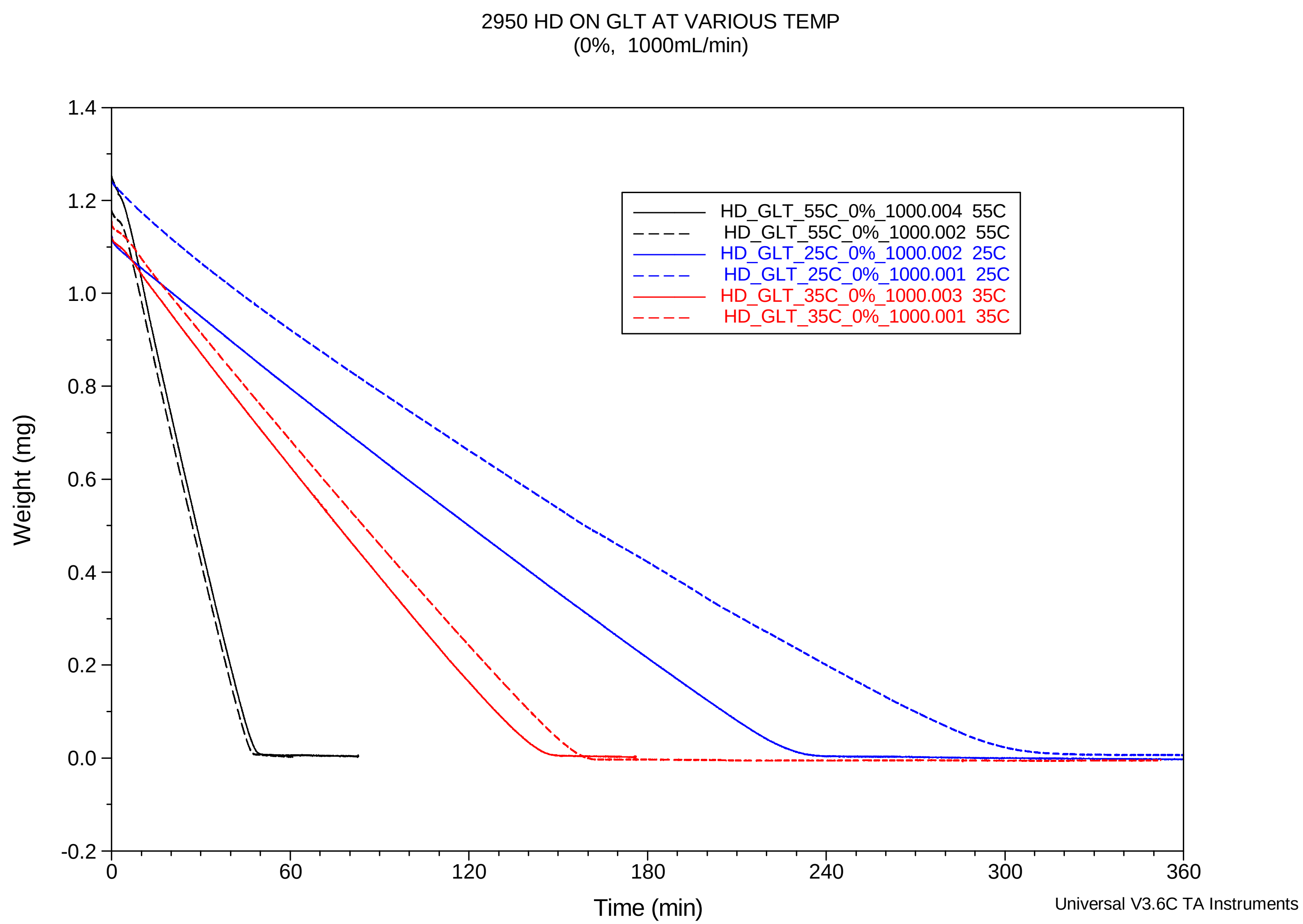


Figure 12. Comparison of HD Evaporation Rate from Glass (TNO) at Various Temperatures:
0% Relative Humidity, 1000 mL/min Flow Rate

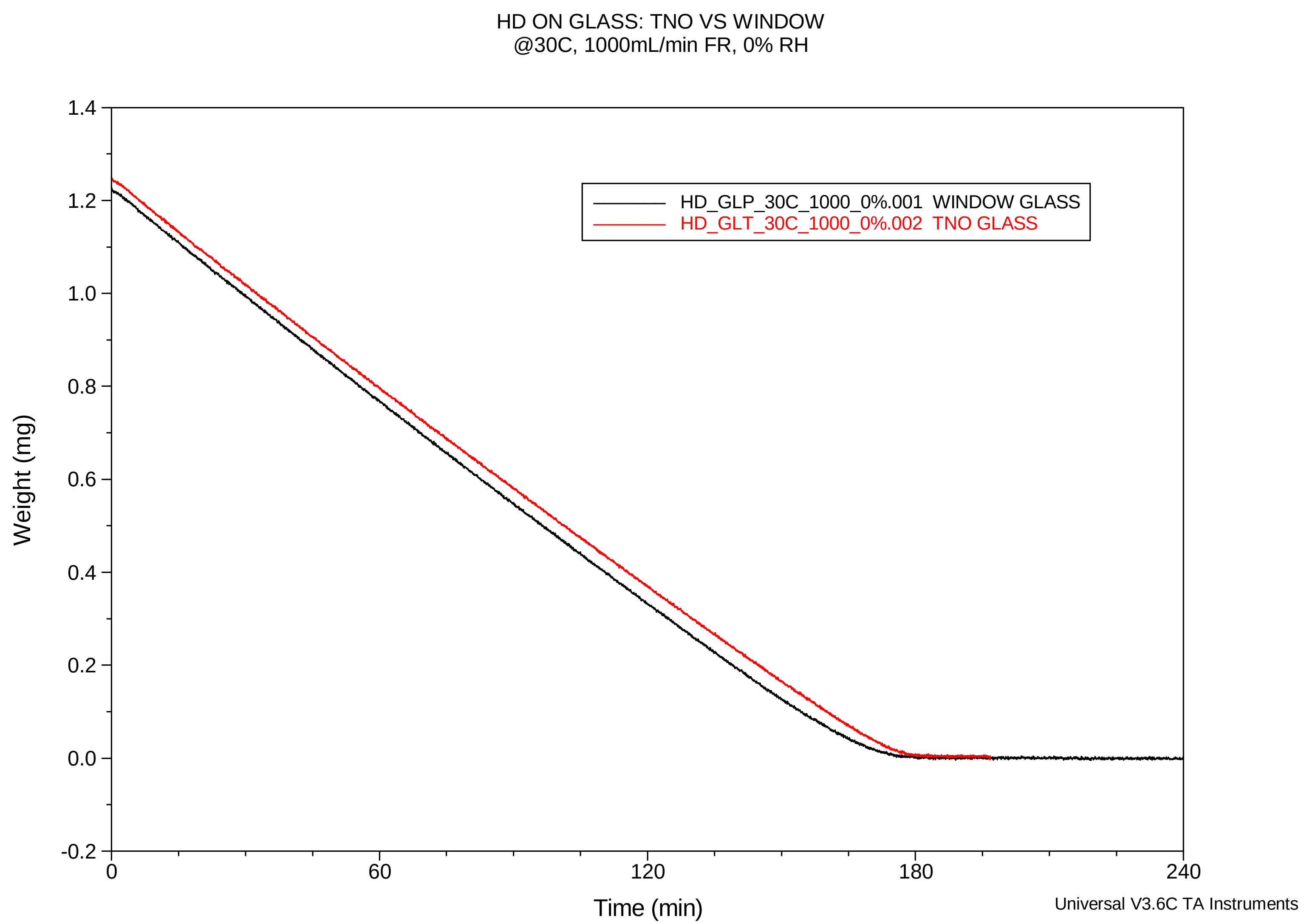


Figure 13. Comparison of HD Evaporation Rate from Glass
TNO Glass vs Window Glass
@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate

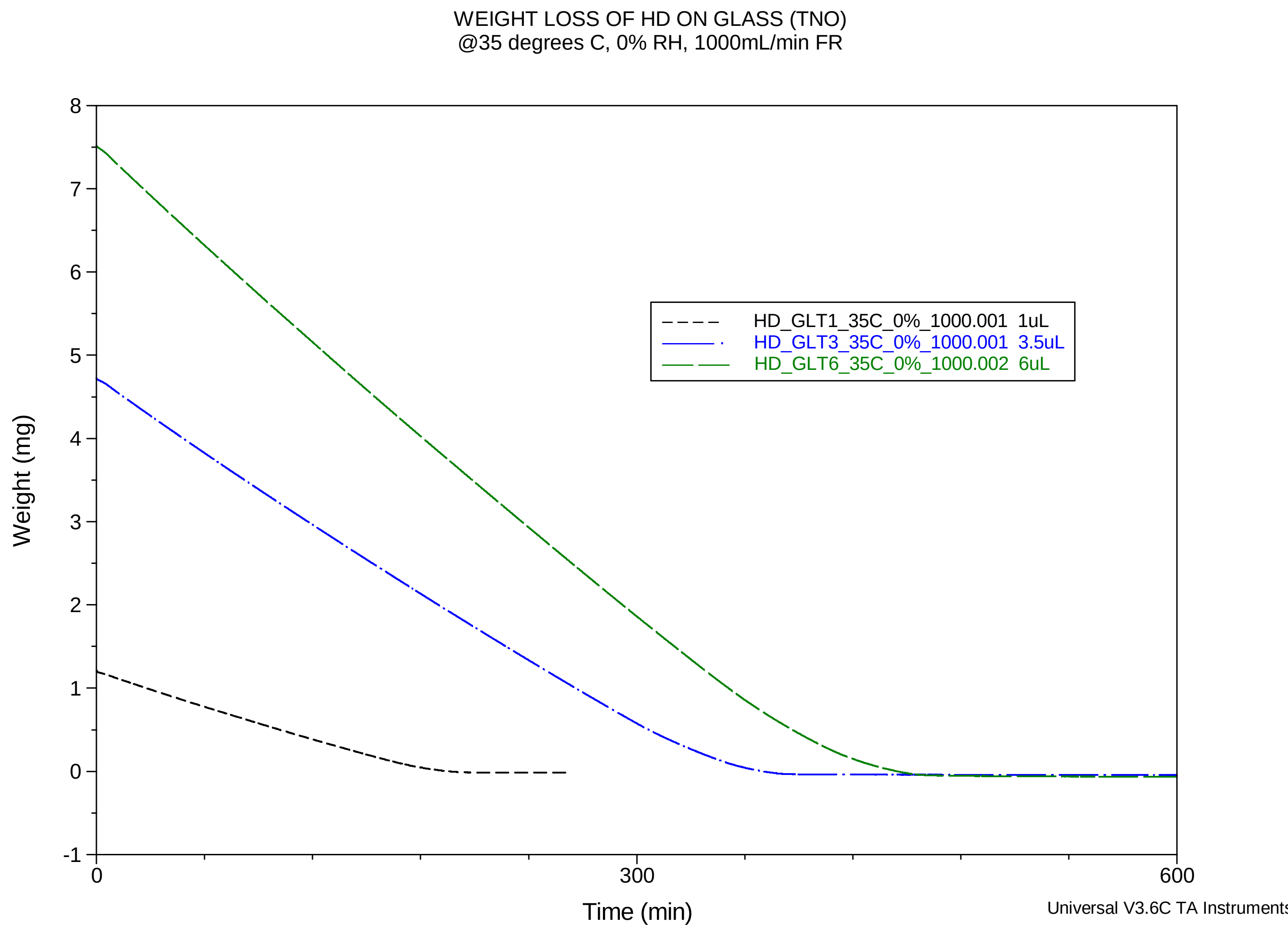


Figure 14. Comparison of HD Evaporation Rate from Glass (TNO):
Drop Size Effect
@35 degrees C, 0% Relative Humidity, 1000 mL/min Flow Rate

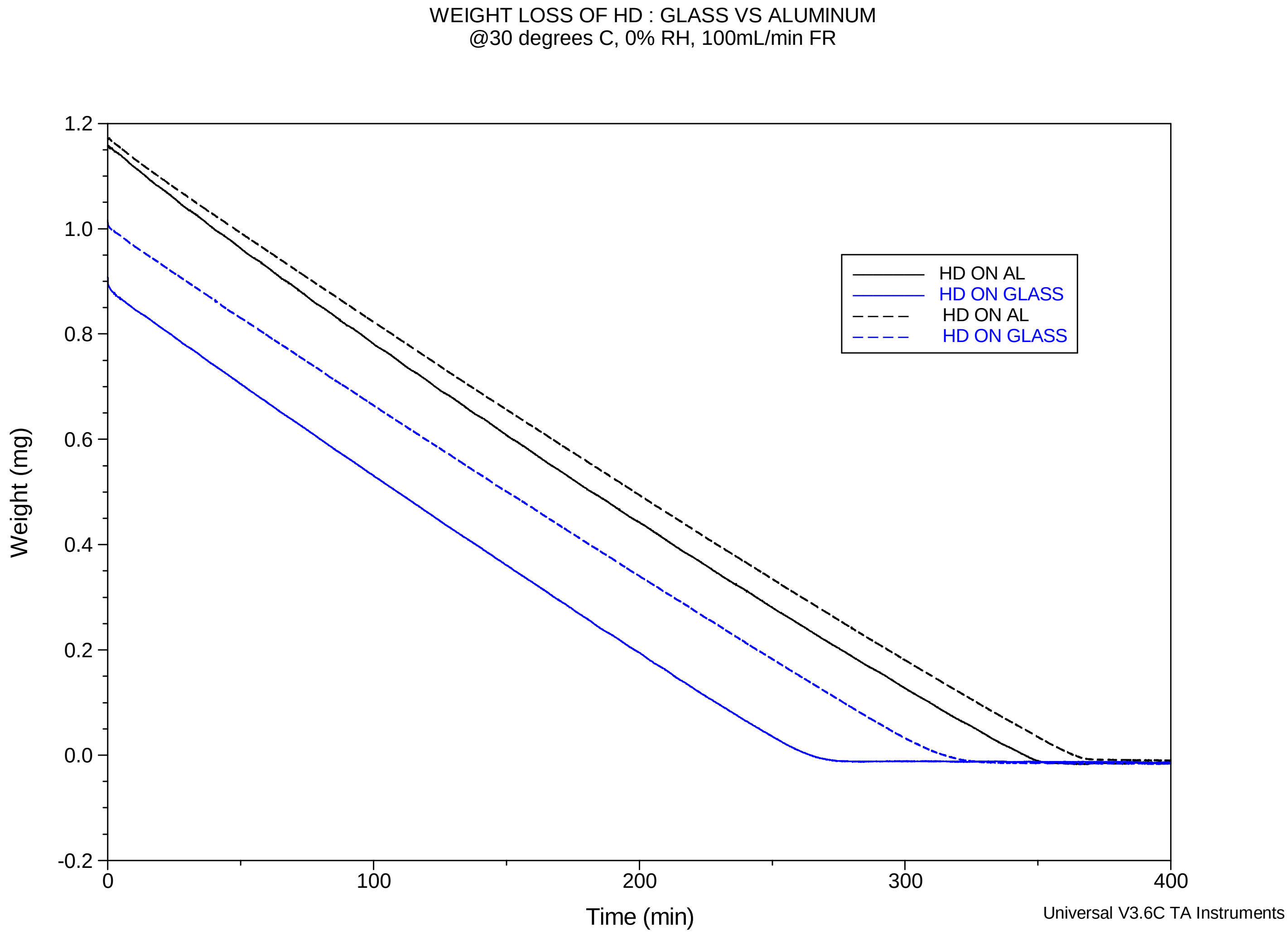


Figure 15. Comparison of HD Evaporation Rate from Glass (window) versus Aluminum: @30 degrees C, 0% Relative Humidity, 100mL/min Flow Rate.

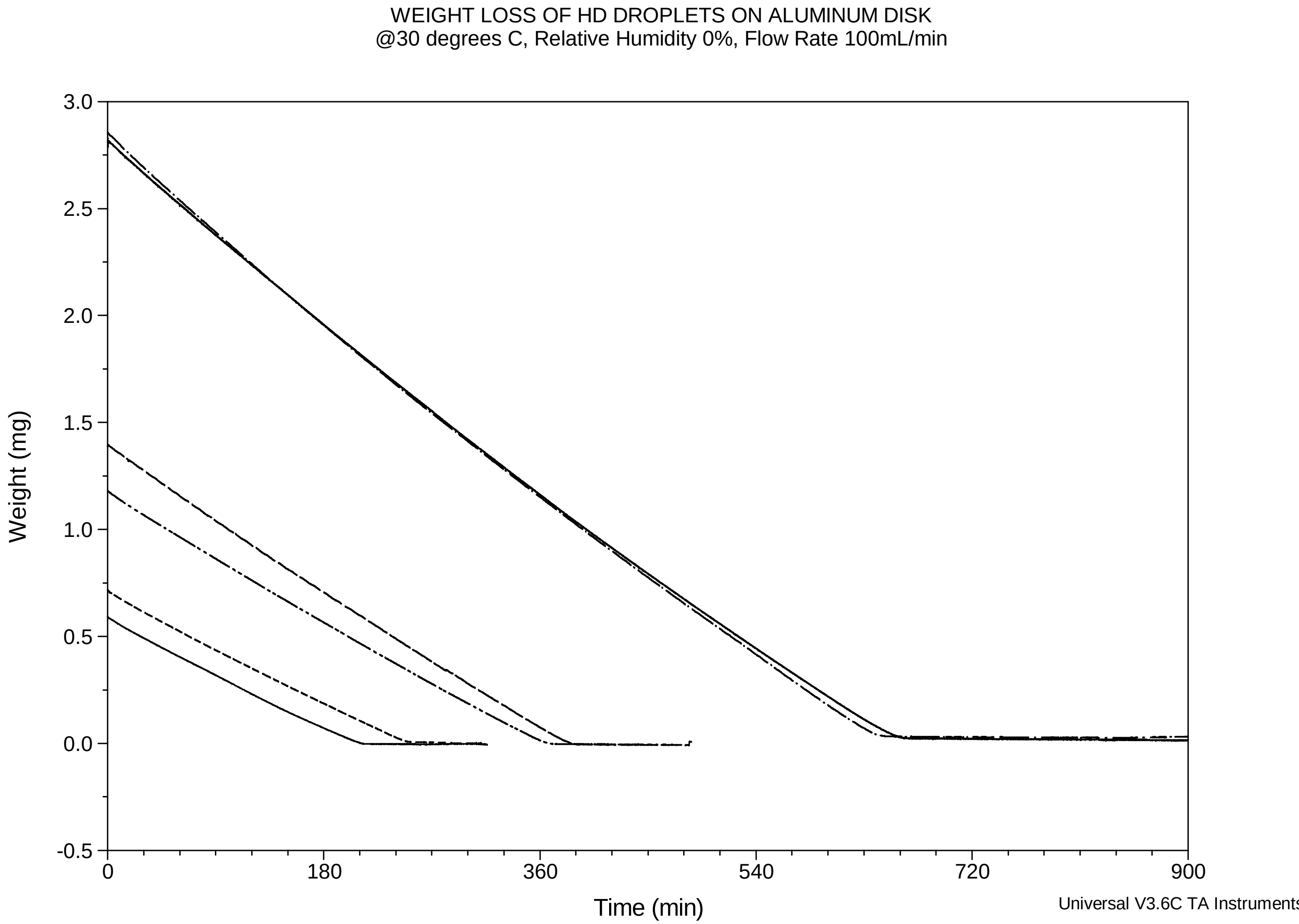


Figure 16. Comparison of HD Evaporation Rate from Aluminum: Drop Size Effect

@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate

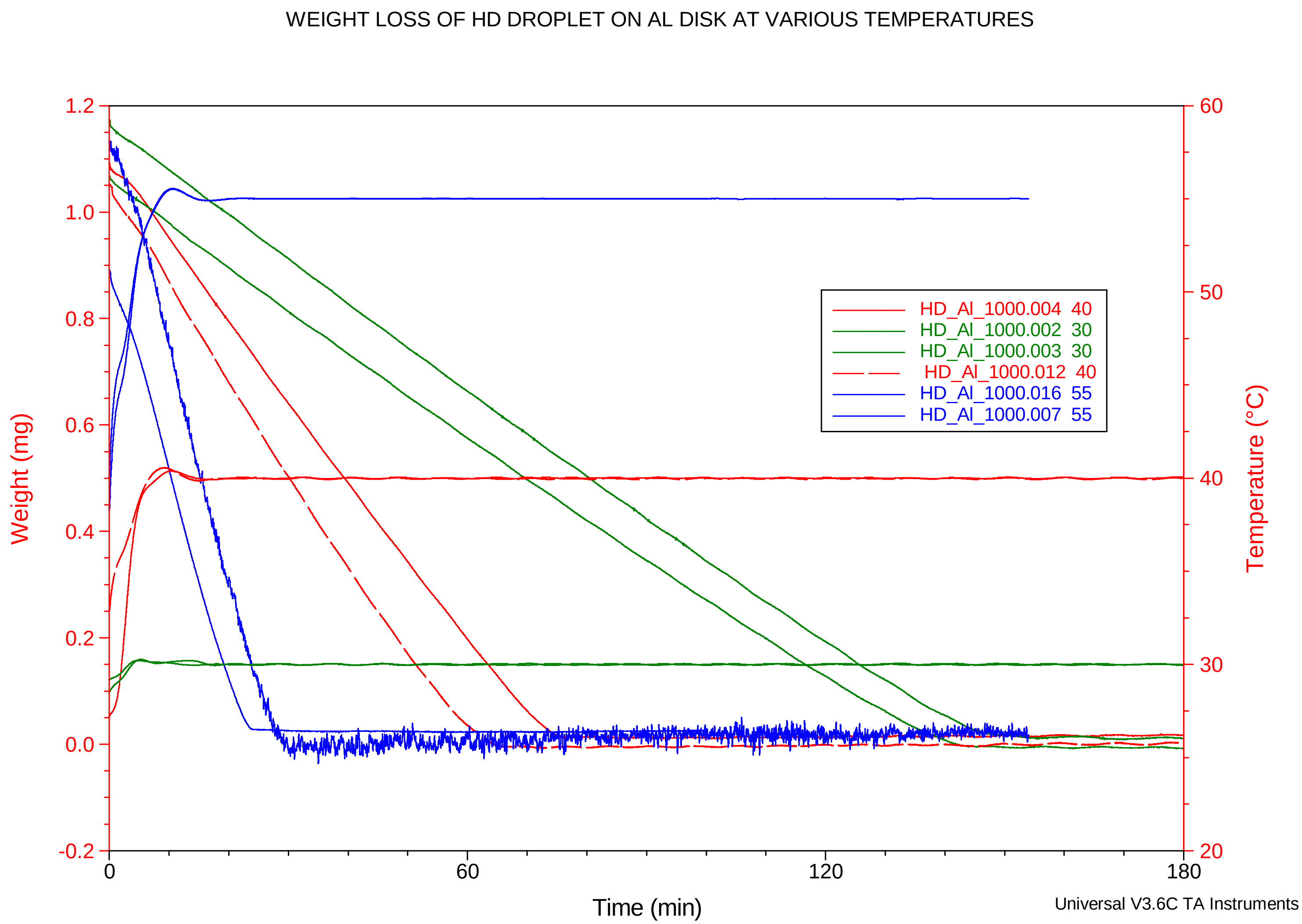


Figure 17. Comparison of HD Evaporation Rate from Aluminum At Various Temperatures: 0% Relative Humidity, 100 mL/min Flow Rate.

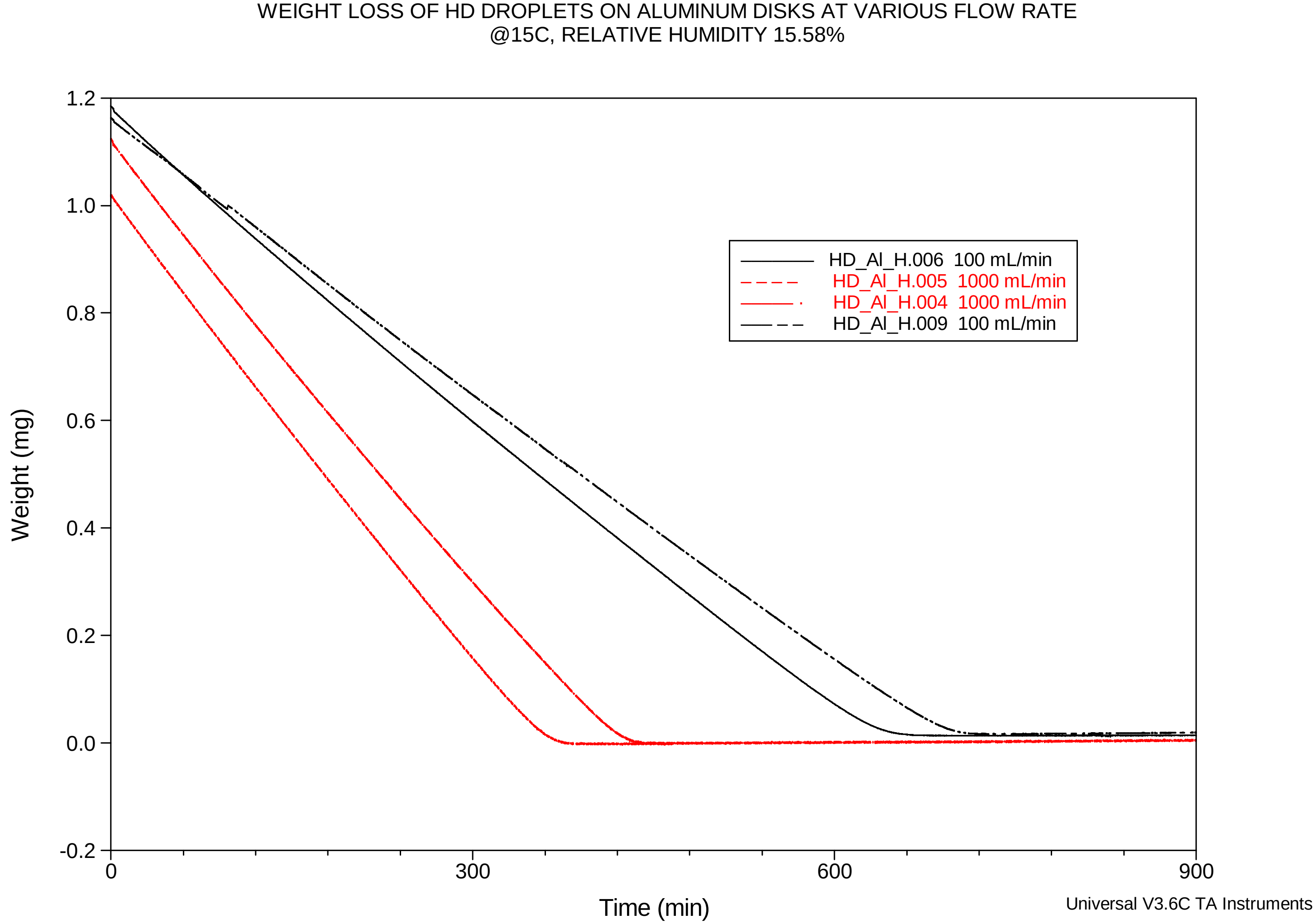


Figure 18. Comparison of HD Evaporation Rate from Aluminum at Various Flow Rates:
@15 degrees C, 15.58% Relative Humidity

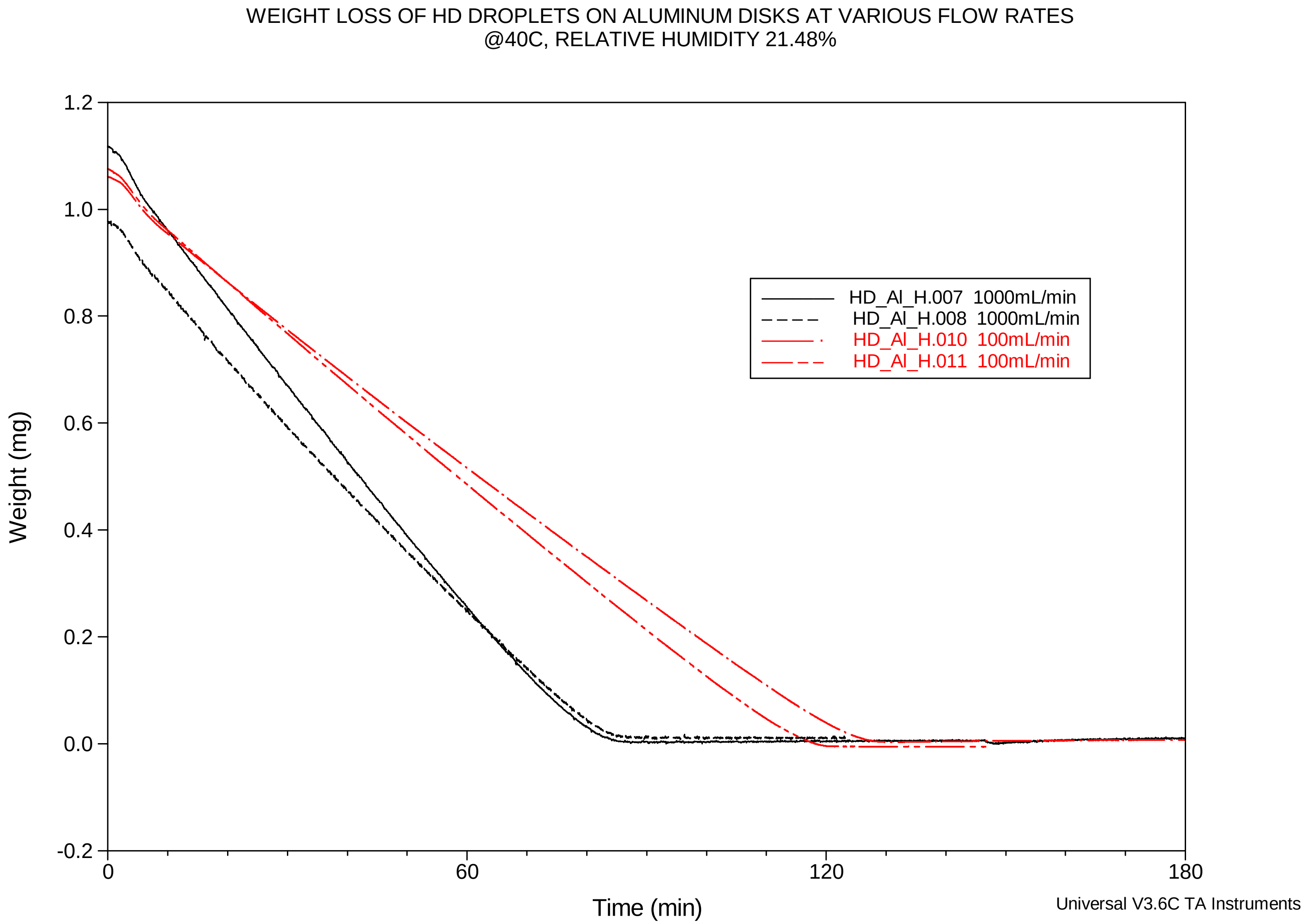


Figure 19. Comparison of HD Evaporation Rate from Aluminum At Various Flow Rates:
@40 degrees C, 21.5% Relative Humidity

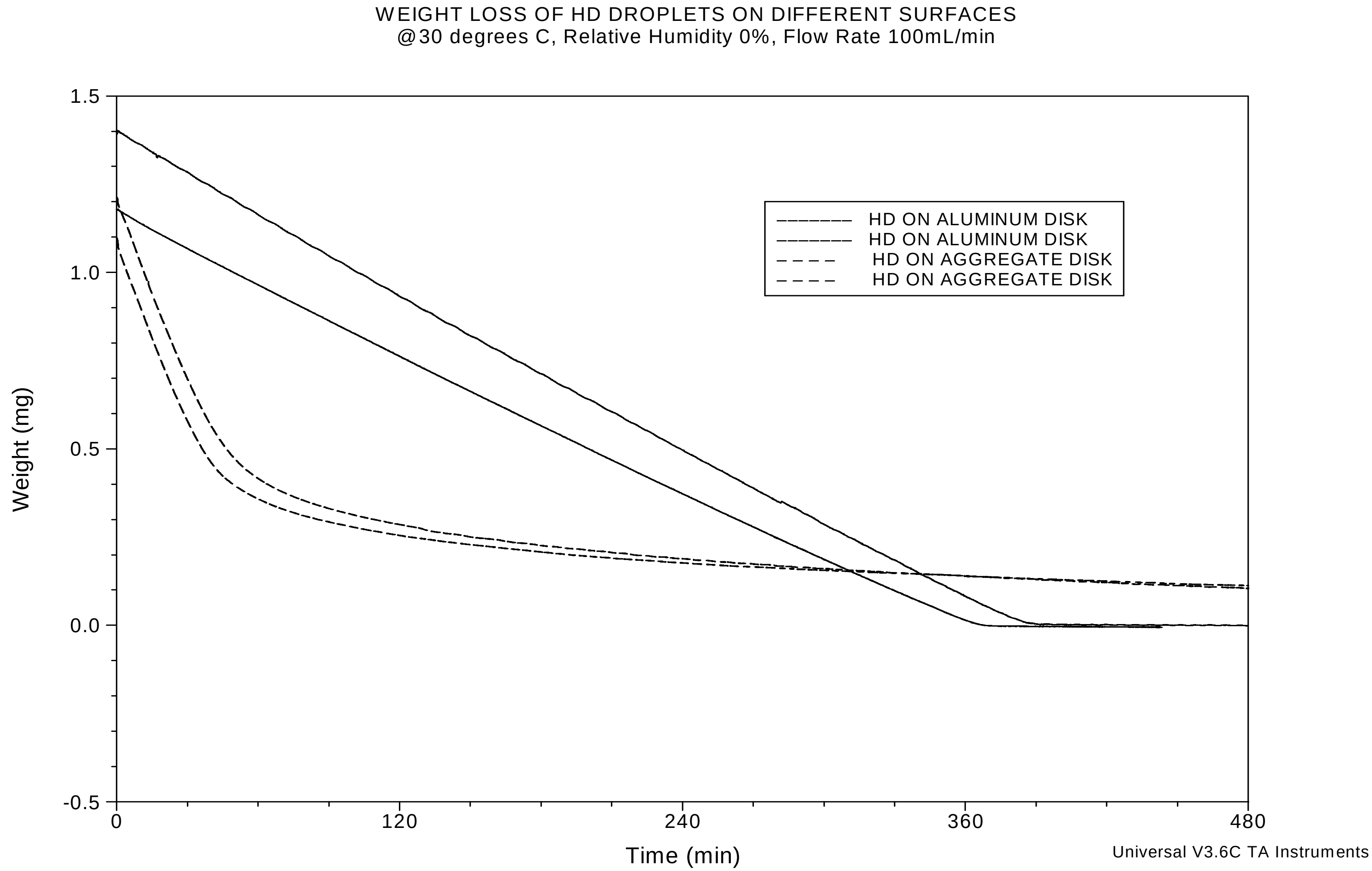


Figure 20. Comparison of HD Evaporation Rate from Aluminum versus Aggregate: @30 degrees C, 0% Relative Humidity, 100mL/min Flow Rate.

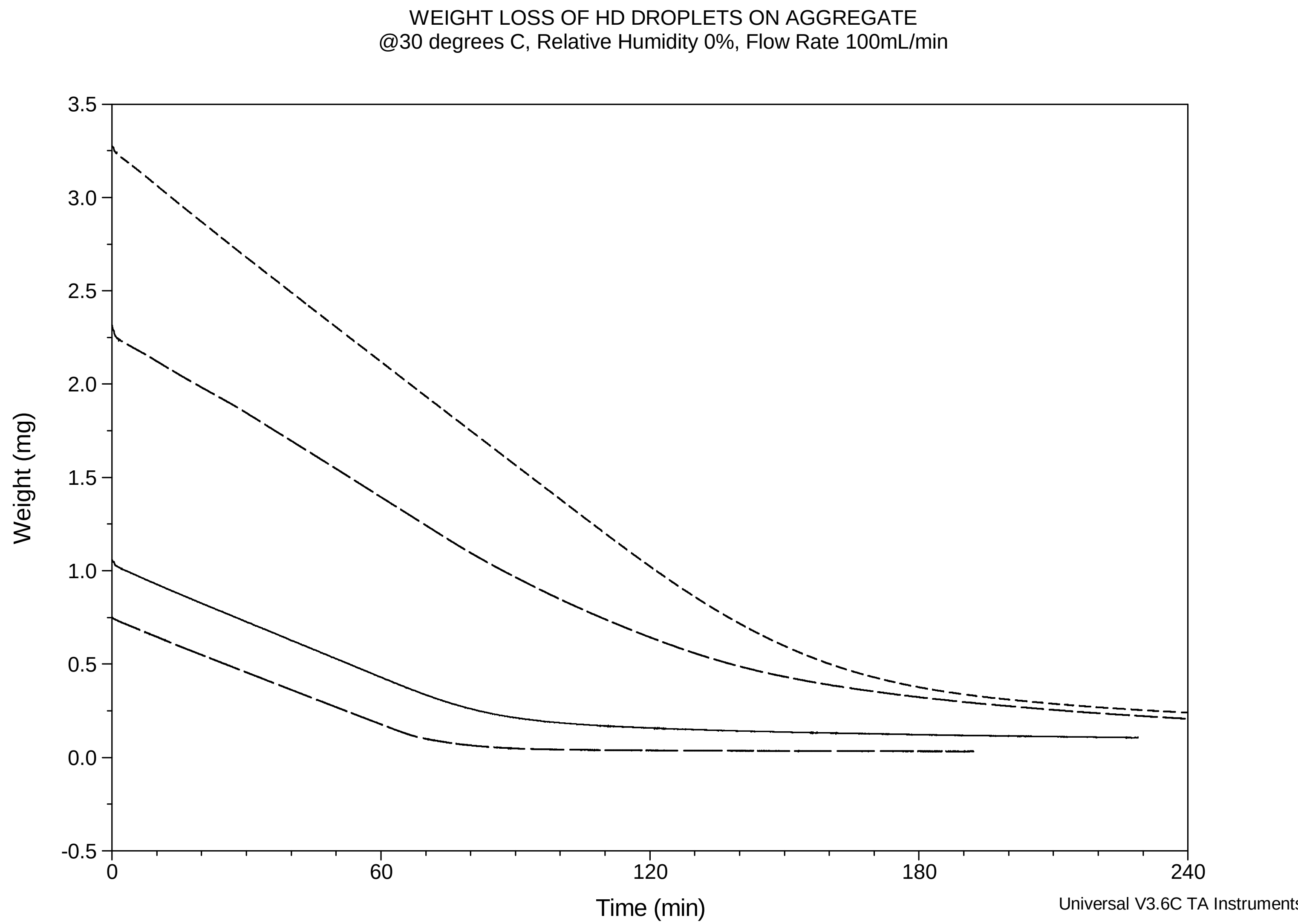


Figure 21. Comparison of HD Evaporation Rate from Aggregate:
Effect of Drop Size
@30 degrees C, 0% Relative Humidity, 100mL/min Flow Rate

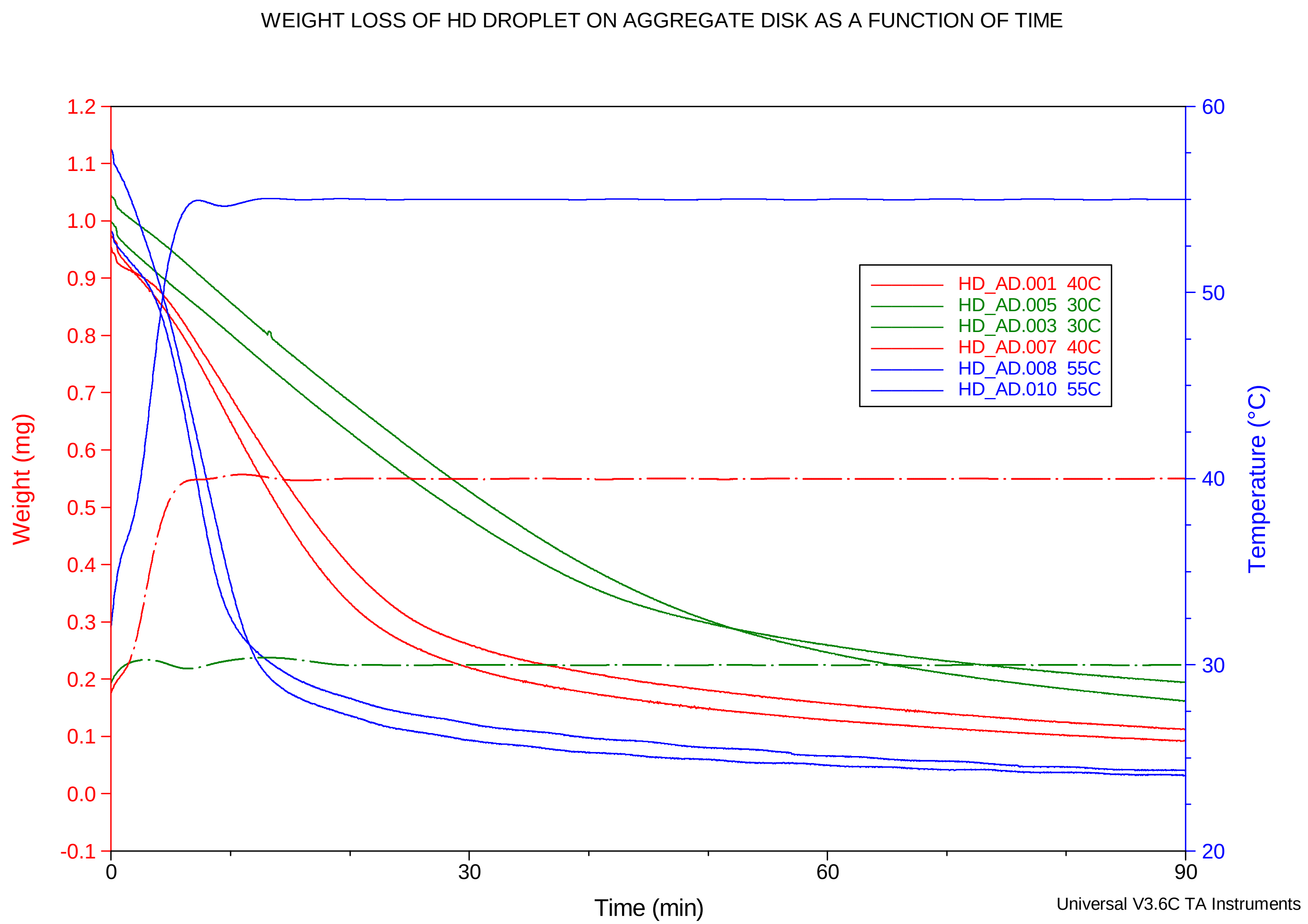


Figure 22. Comparison of HD Evaporation Rate from Aggregate
At Various Temperatures:
0% Relative Humidity, 100mL/min Flow Rate.

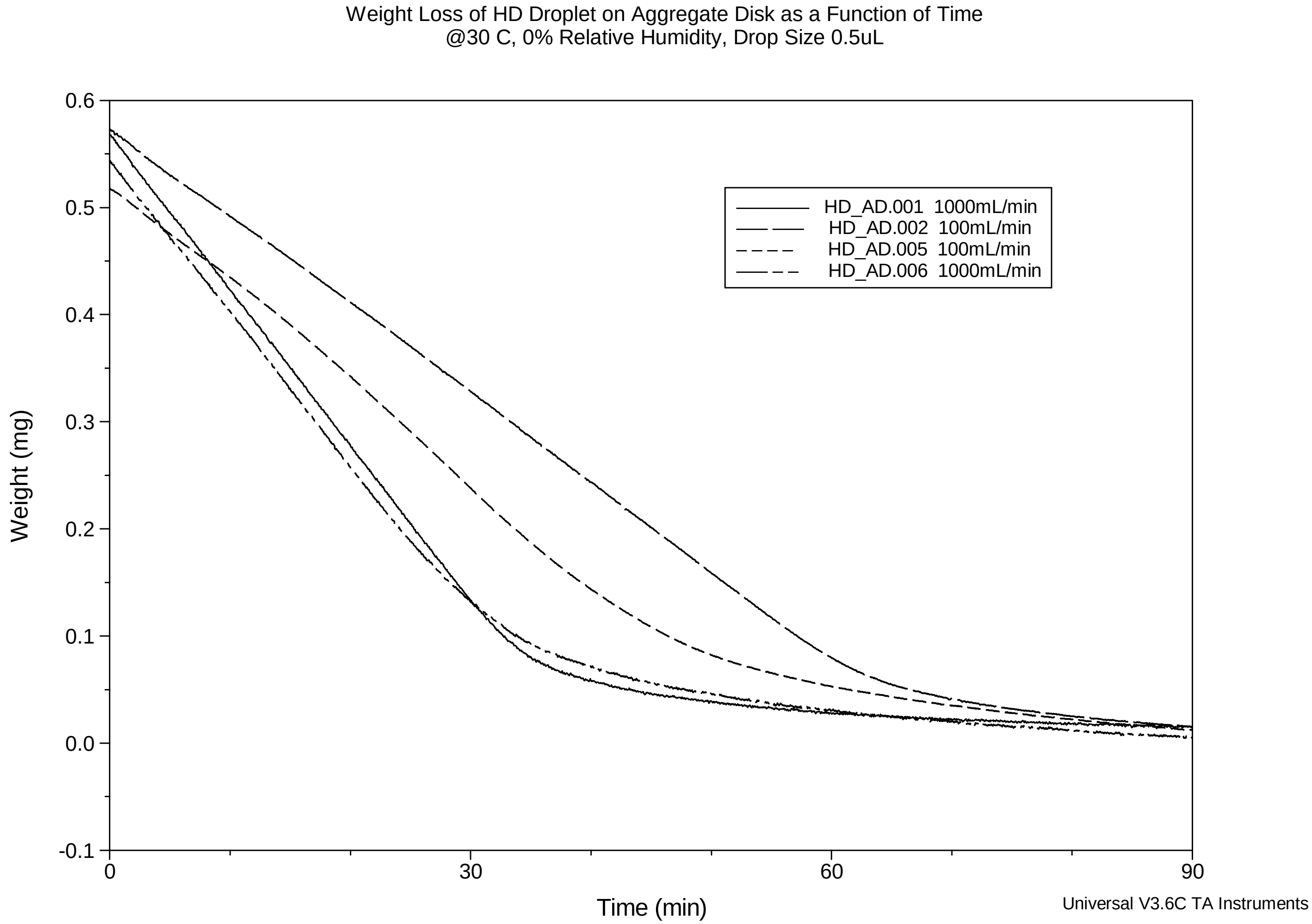


Figure 23. Comparison of HD Evaporation Rate from Aggregate at Various Flow Rates:
@30 degrees C, 0% Relative Humidity

Summary Table

Fig #	Surface	Experimental Conditions				Comparison
		Temp (C)	Rel Humidity (%)	Flow Rate (mL/min)	Drop size (uL)	
7	Glass, cover	30	0	100	0.91	Cleaned vs Uncleaned
8	Glass, window	40	0	V	0.91	Various Flow Rates
9	Glass, window	V	0	100	0.91	Various Temp
10	Glass, window	30	0	100	V	Various Drop Sizes
11	Glass, window	40	V	500	0.91	Relative Humidity
12	Glass, TNO	V	0	1000	0.91	Various Temp
13	Glass	30	0	100	0.91	Surface
14	Glass, TNO	35	0	1000	V	Various Drop Sizes
15	Glass & Al	30	0	100	1	Surface
16	Aluminum	30	0	100	V	Various Drop Sizes
17	Aluminum	V	0	100	1	Various Temp
18	Aluminum	15	15.6	V	1	Various Flow Rates
19	Aluminum	40	21.5	V	1	Various Flow Rates
20	Al & Aggregate	30	0	100	1	Surface
21	Aggregate	30	0	100	V	Various Drop Sizes
22	Aggregate	V	0	100	1	Various Temp
23	Aggregate	30	0	V	0.5	Various Flow Rates

Summary

A preliminary evaluation indicates;

- Rates apparently follow zero-order, film evaporation on inert, non-porous surfaces (Glass and Aluminum).
- Time to complete evaporation increased systematically with drop-size.
- Flow rate, Temperature influence evaporation rate of HD as expected.
- Humidity has no apparent effect on evaporation rate of HD.
- Nitric acid/hexane cleaning of glass has a small effect on evaporation rate of HD.
- Initial evaporation rate of CWA on Concrete Aggregates was more rapid than that on Aluminum Disks, probably due to the Wetted Surface Area (Spread Factor).

ACKNOWLEDGEMENTS

The authors wish to acknowledge managerial support by Dr. H. Durst and Dr. J. Savage, ECBC.

BACKUP SLIDES

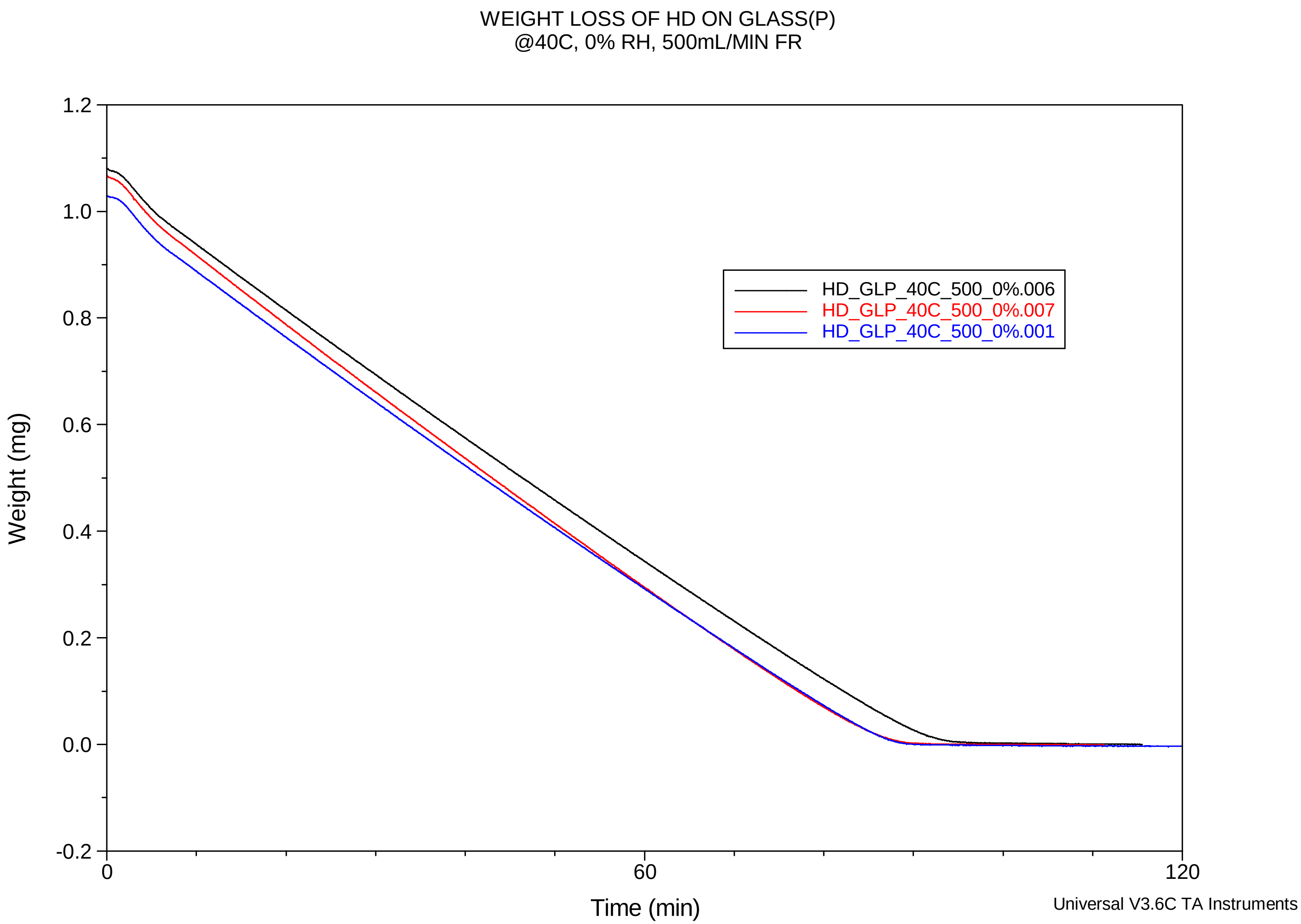


Figure. HD Evaporation Rate from Glass (Window):
@40 degrees C, 0% Relative Humidity, 500 mL/min Flow Rate

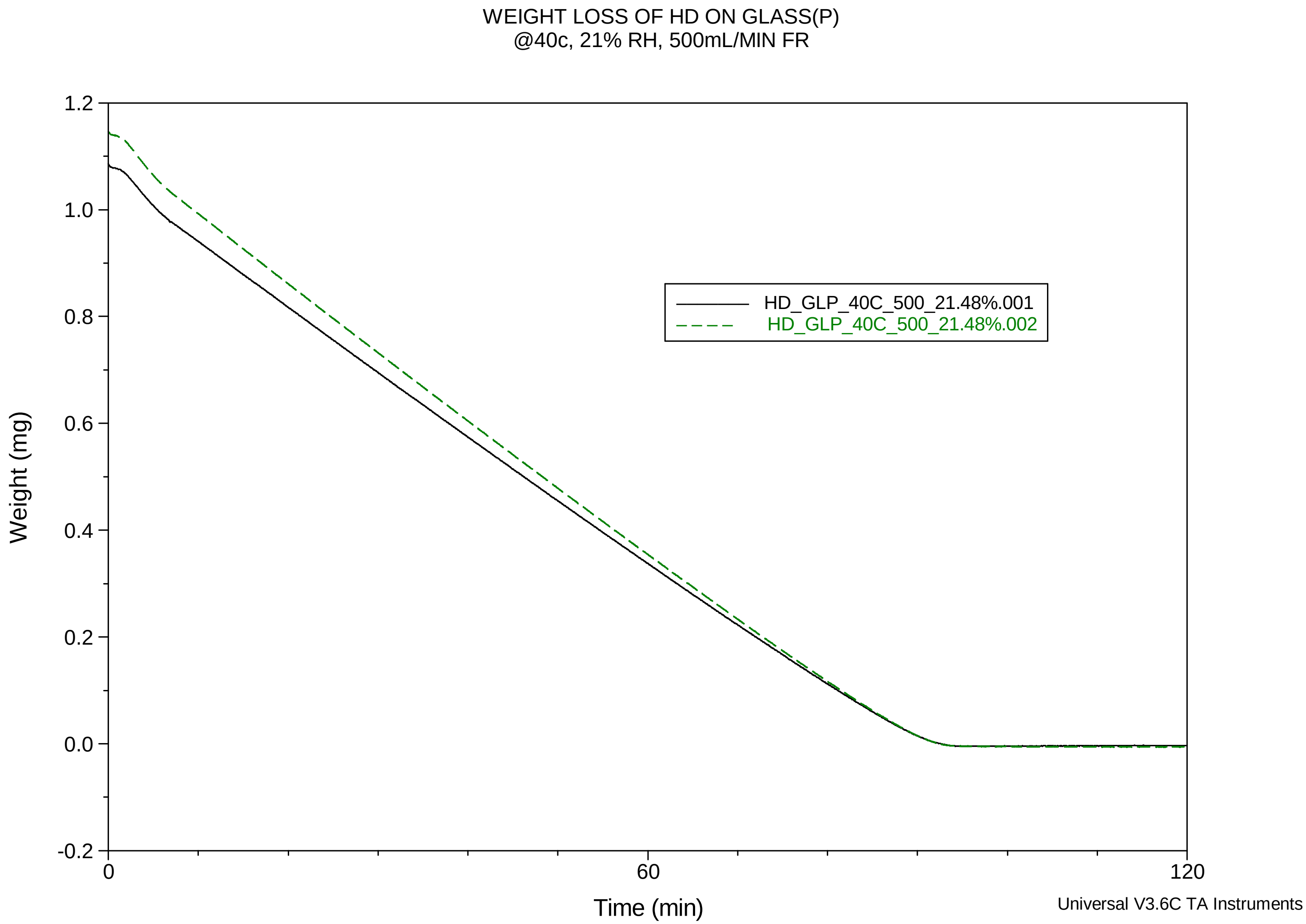


Figure. HD Evaporation Rate from Glass (Window):
@40 degrees C, 21.5% Relative Humidity, 500 mL/min Flow Rate

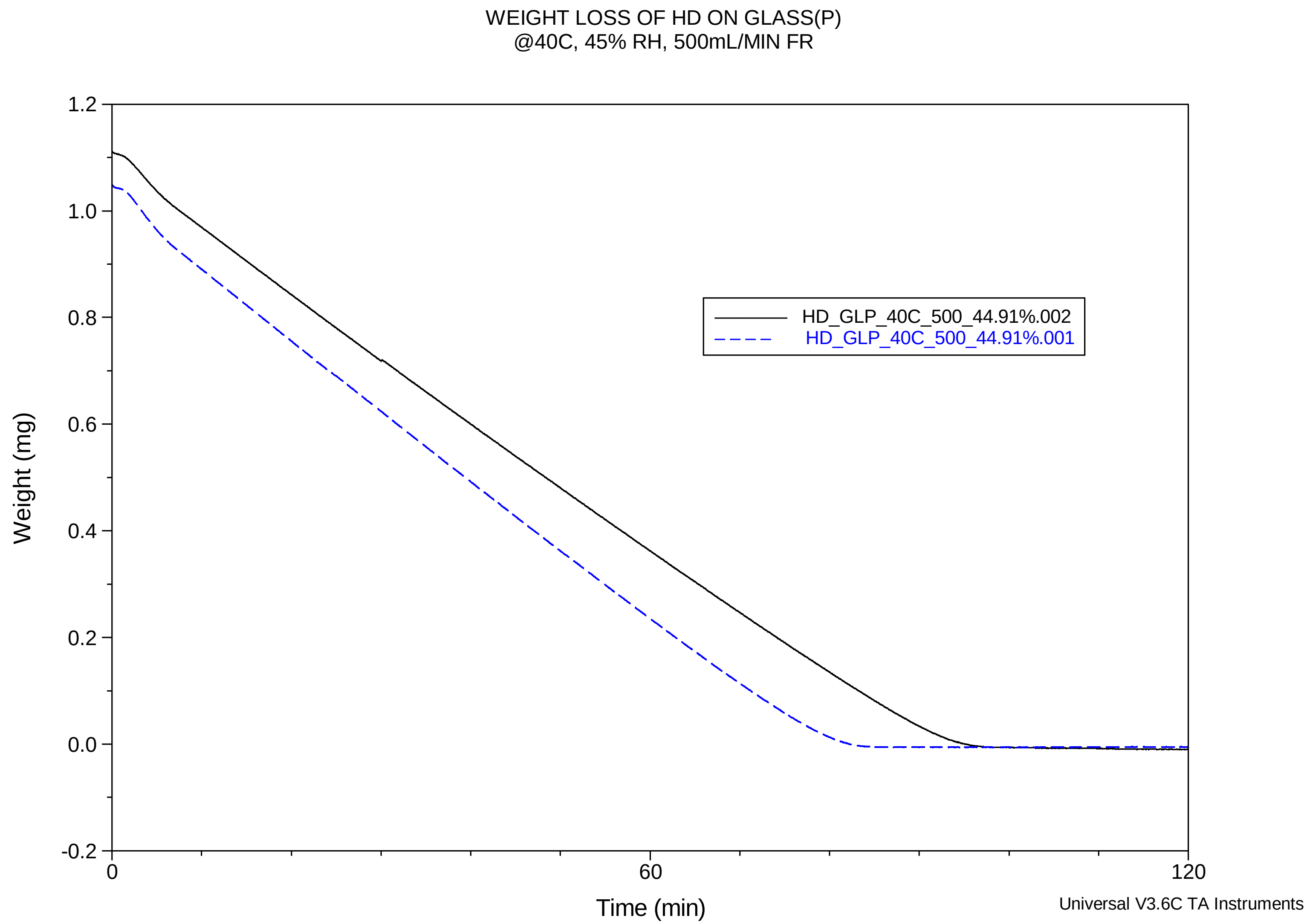


Figure. HD Evaporation Rate from Glass (Window):
@40 degrees C, 44.9% Relative Humidity, 500 mL/min Flow Rate

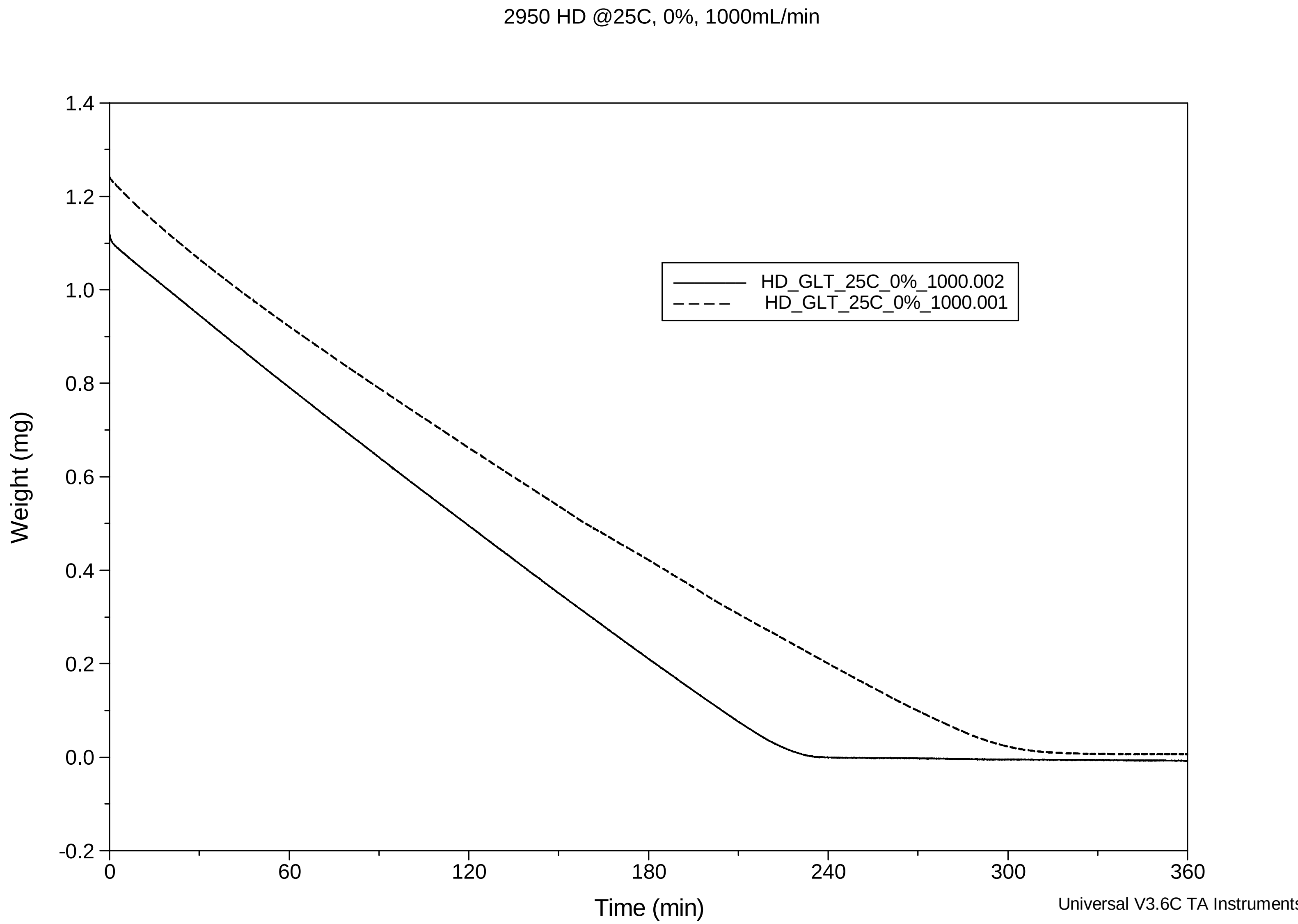


Figure. HD Evaporation Rate from Glass (TNO):
@25 degrees C, 0% Relative Humidity, 1000 mL/min Flow Rate

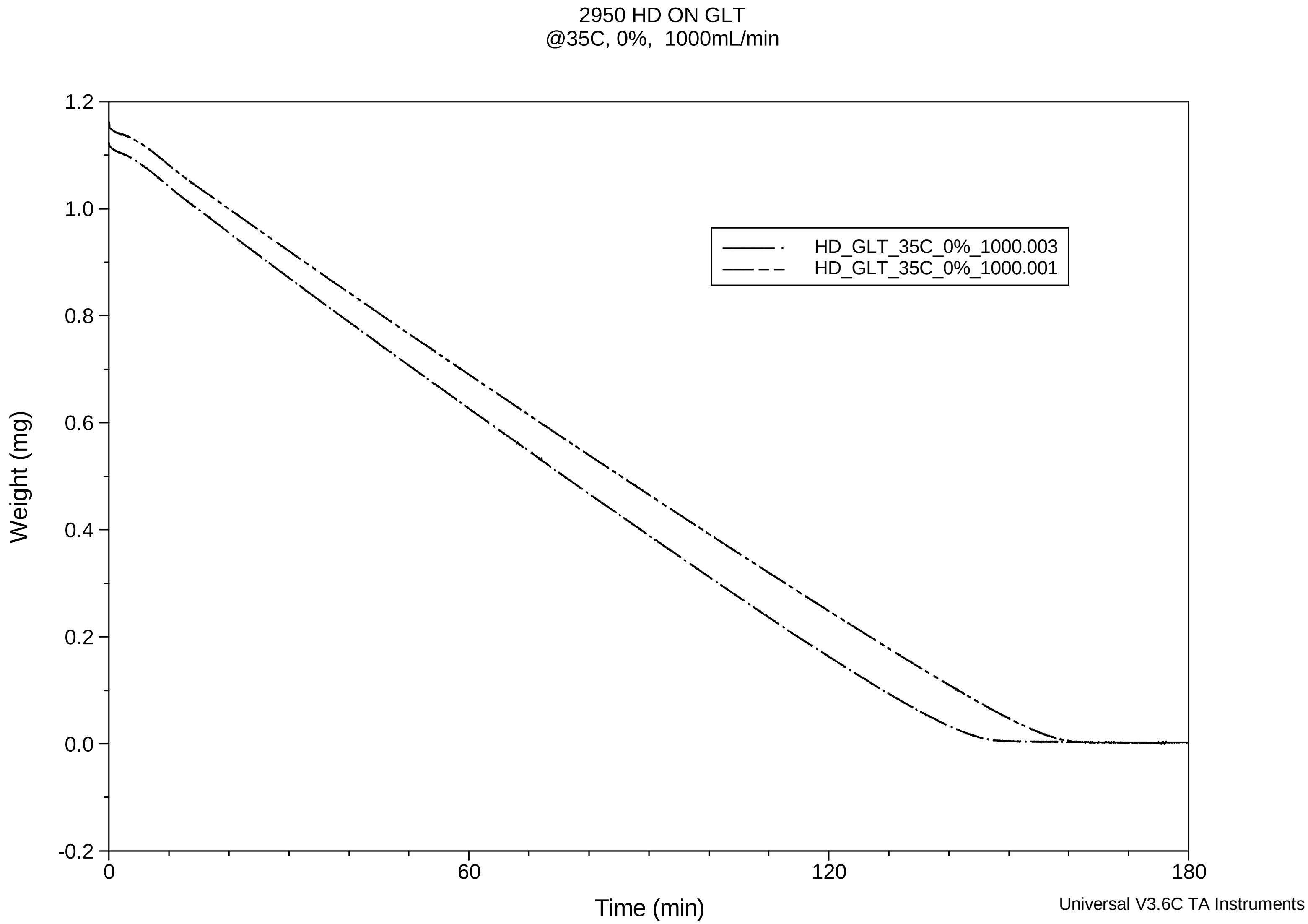


Figure. HD Evaporation Rate from Glass (TNO):
@35 degrees C, 0% Relative Humidity, 1000 mL/min Flow Rate

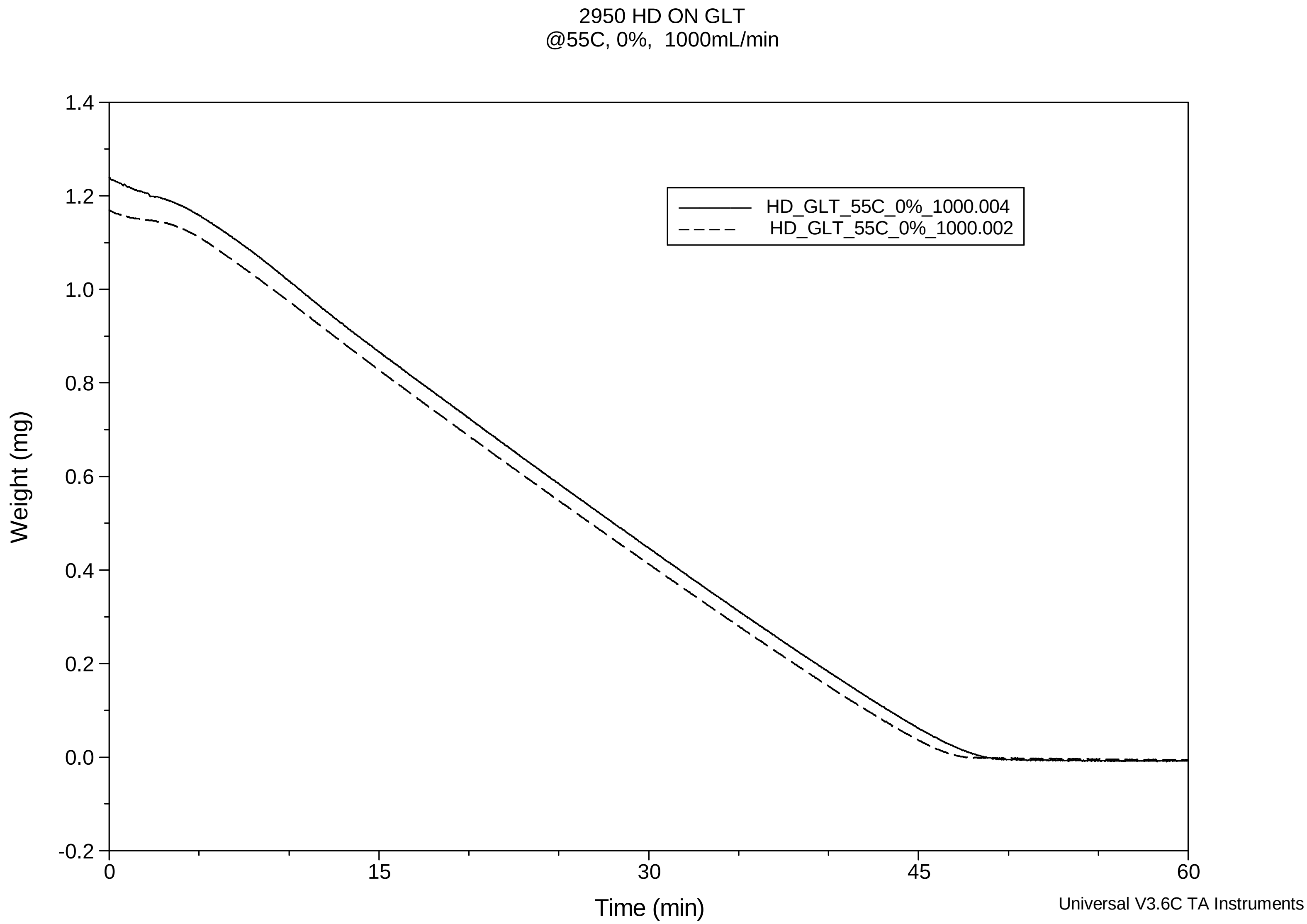


Figure. HD Evaporation Rate from Glass (TNO):
@55 degrees C, 0% Relative Humidity, 1000 mL/min Flow Rate

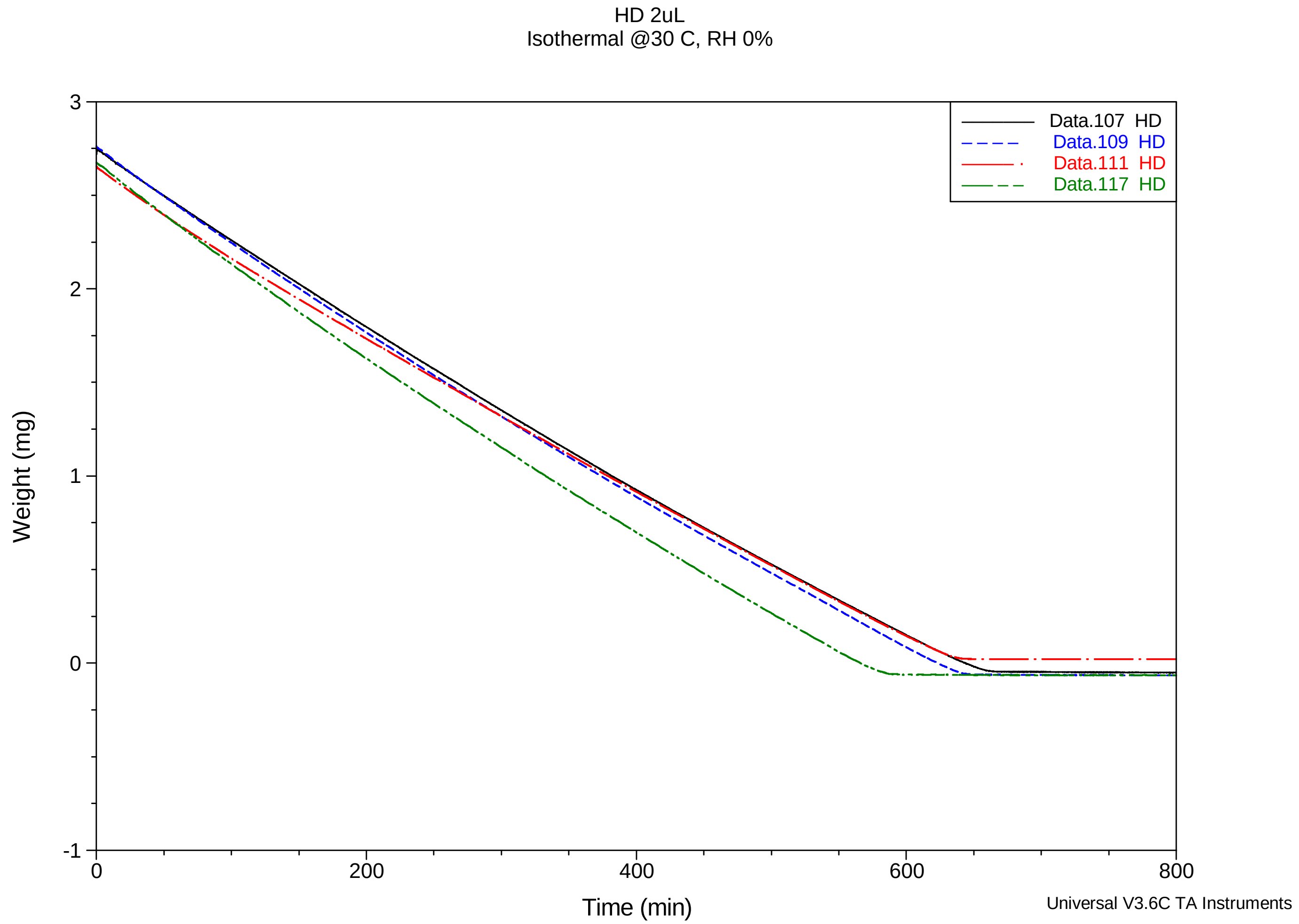


Figure. HD Evaporation Rate from Aluminum:
@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate.

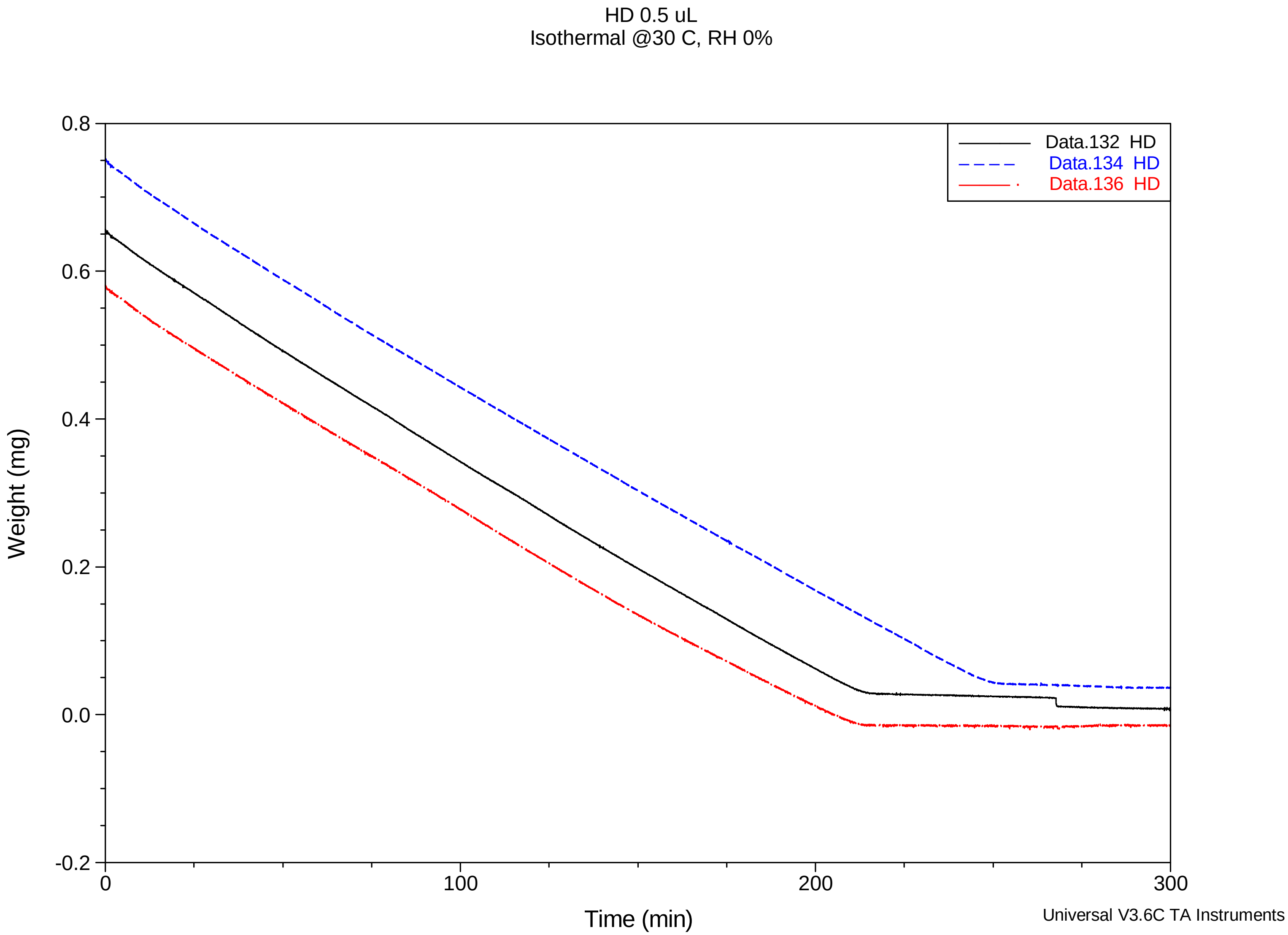
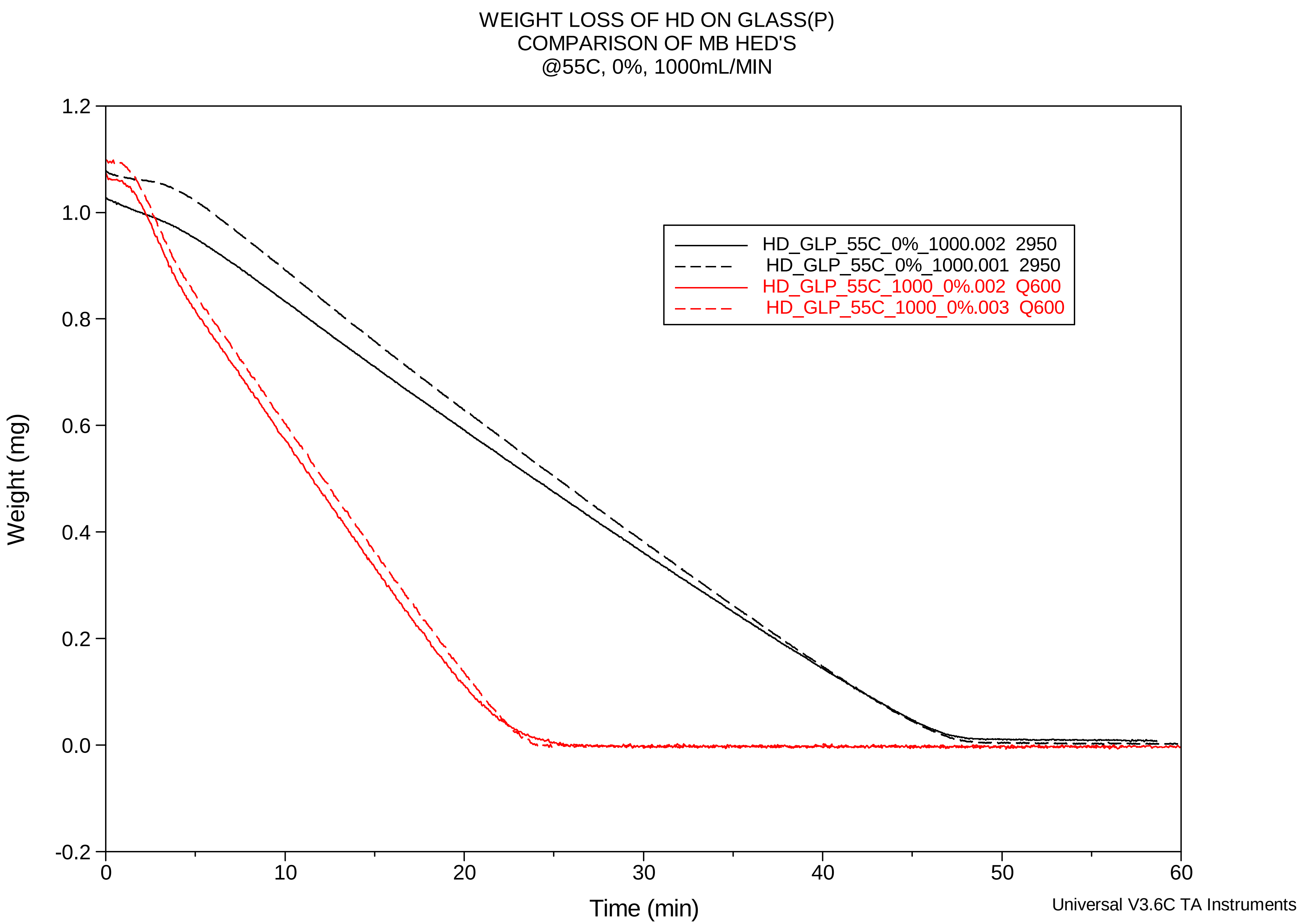


Figure. HD Evaporation Rate from Aluminum:
@30 degrees C, 0% Relative Humidity, 100 mL/min Flow Rate.


WEIGHT LOSS OF HD ON GLASS(P)
COMPARISON OF MB HED'S
@55C, 0%, 1000mL/MIN
HD_GLP_55C_0%_1000.002 2950
HD_GLP_55C_0%_1000.001 2950
HD_GLP_55C_1000_0%.002 Q600
HD_GLP_55C_1000_0%.003 Q600
Weight (mg)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
0
10
20
30
40
50
60
Time (min)
Universal V3.6C TA Instruments

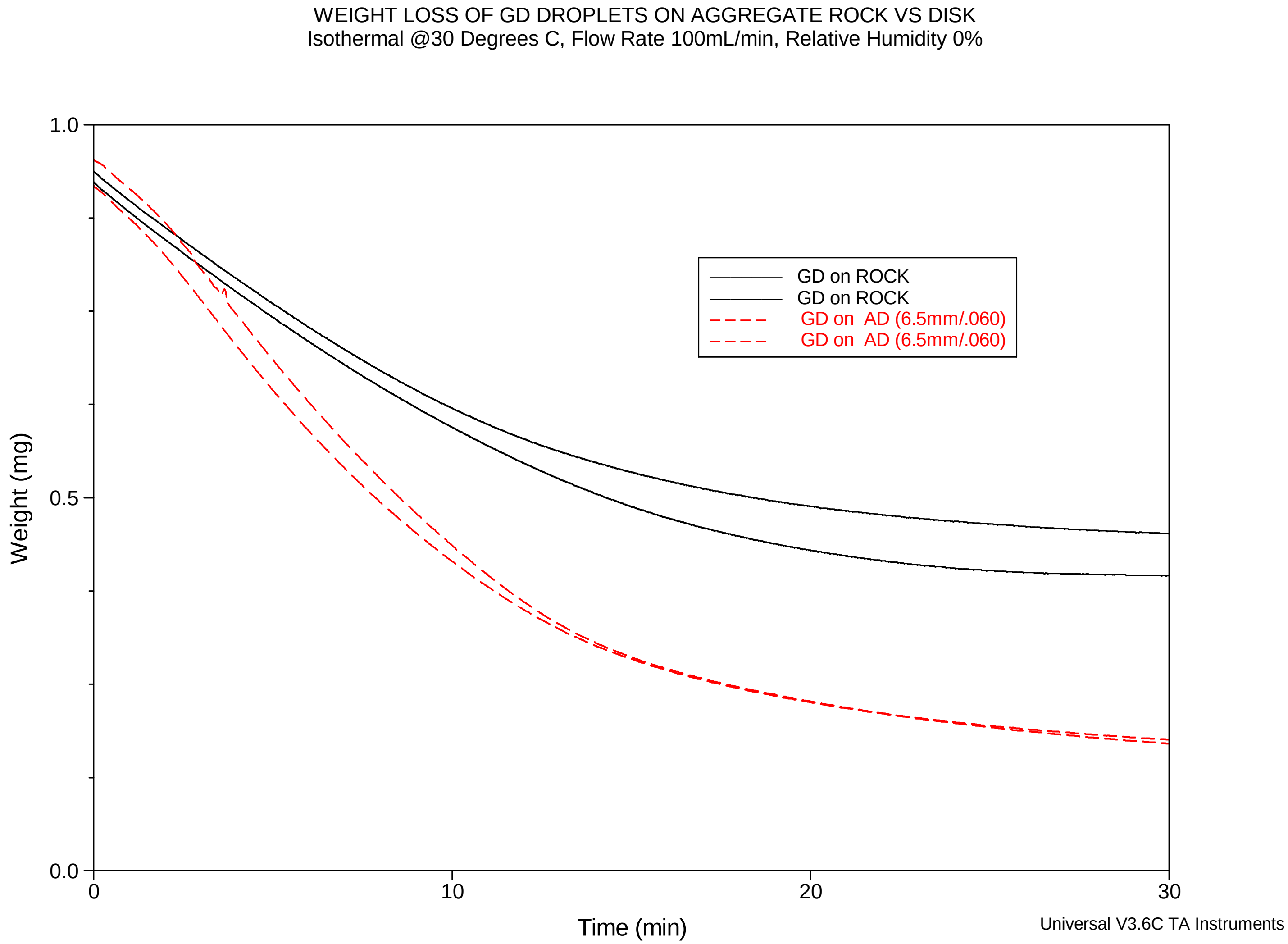


Figure. WEIGHT LOSS OF GD DROPLETS ON AGGREGATE ROCK VS DISK
Isothermal @ 30 Degrees C, Relative humidity 0%, Flow Rate 100mL/min

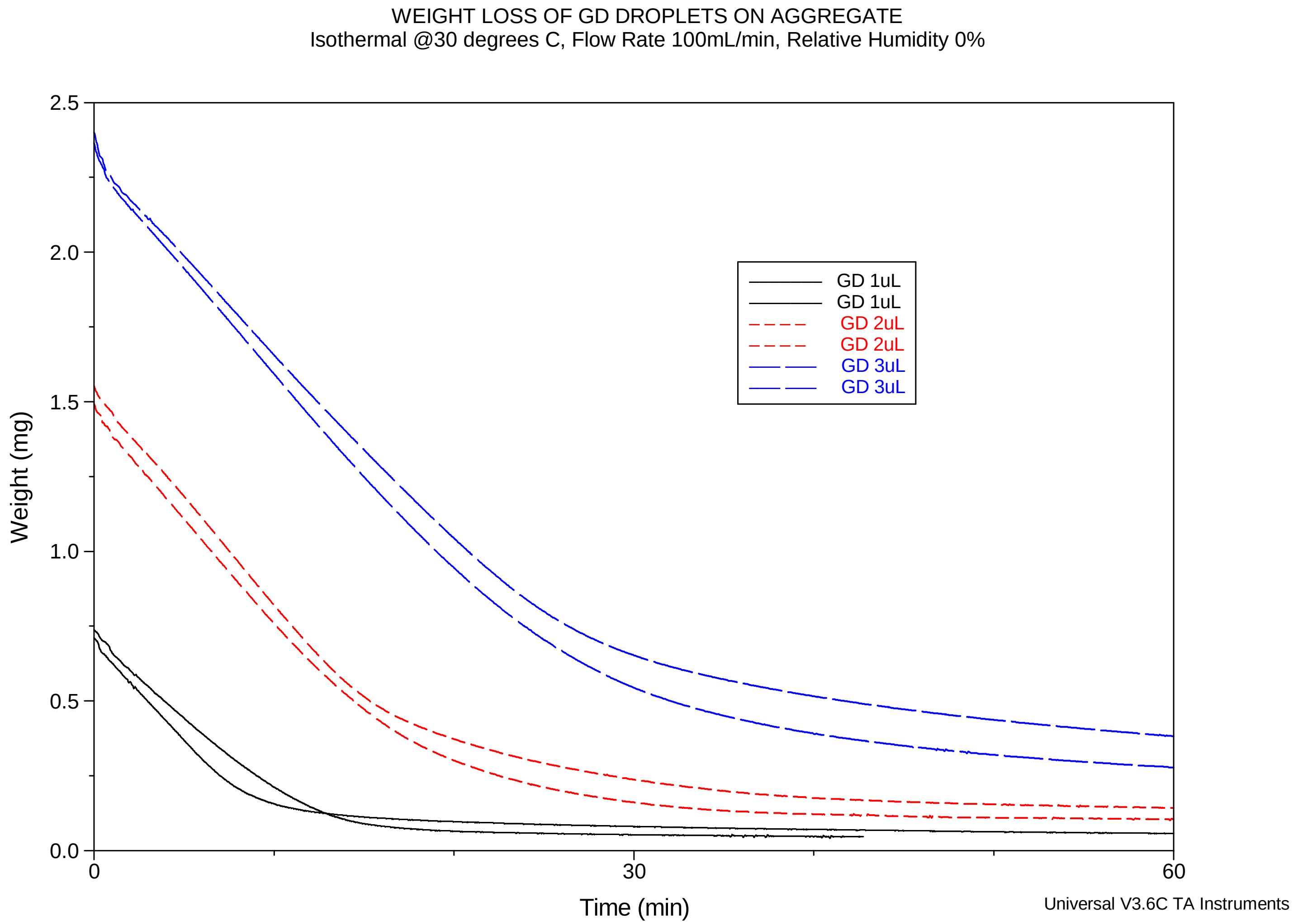


Figure. WEIGHT LOSS OF GD DROPLETS ON AGGREGATE
Isothermal @ 30 Degrees C, Relative humidity 0%, Flow Rate 100mL/min

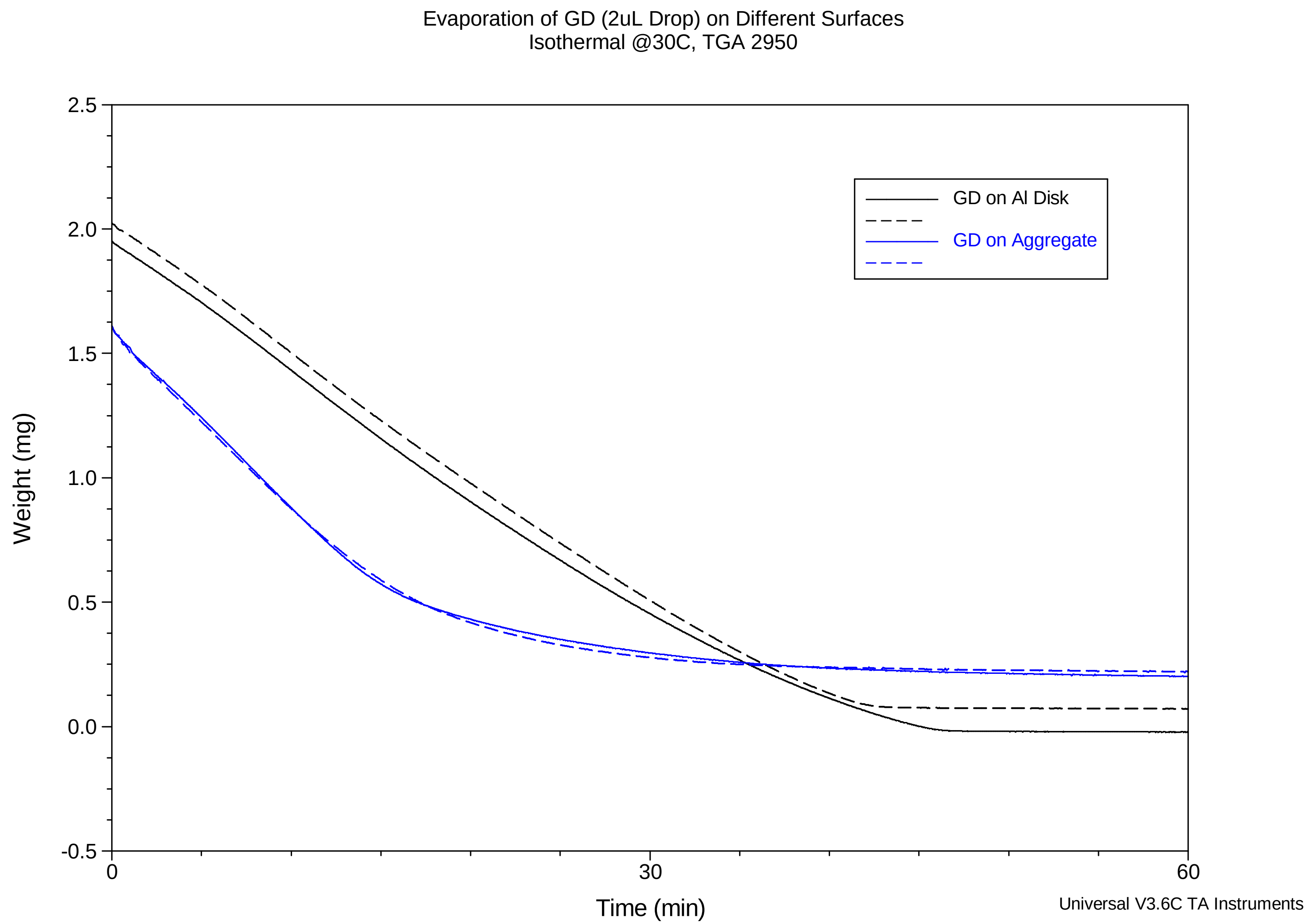


Figure. WEIGHT LOSS OF GD ON ALUMINUM DISKS vs AGGREGATE
Isothermal @ 30 Degrees C, Relative humidity 0%, Flow Rate 100mL/min

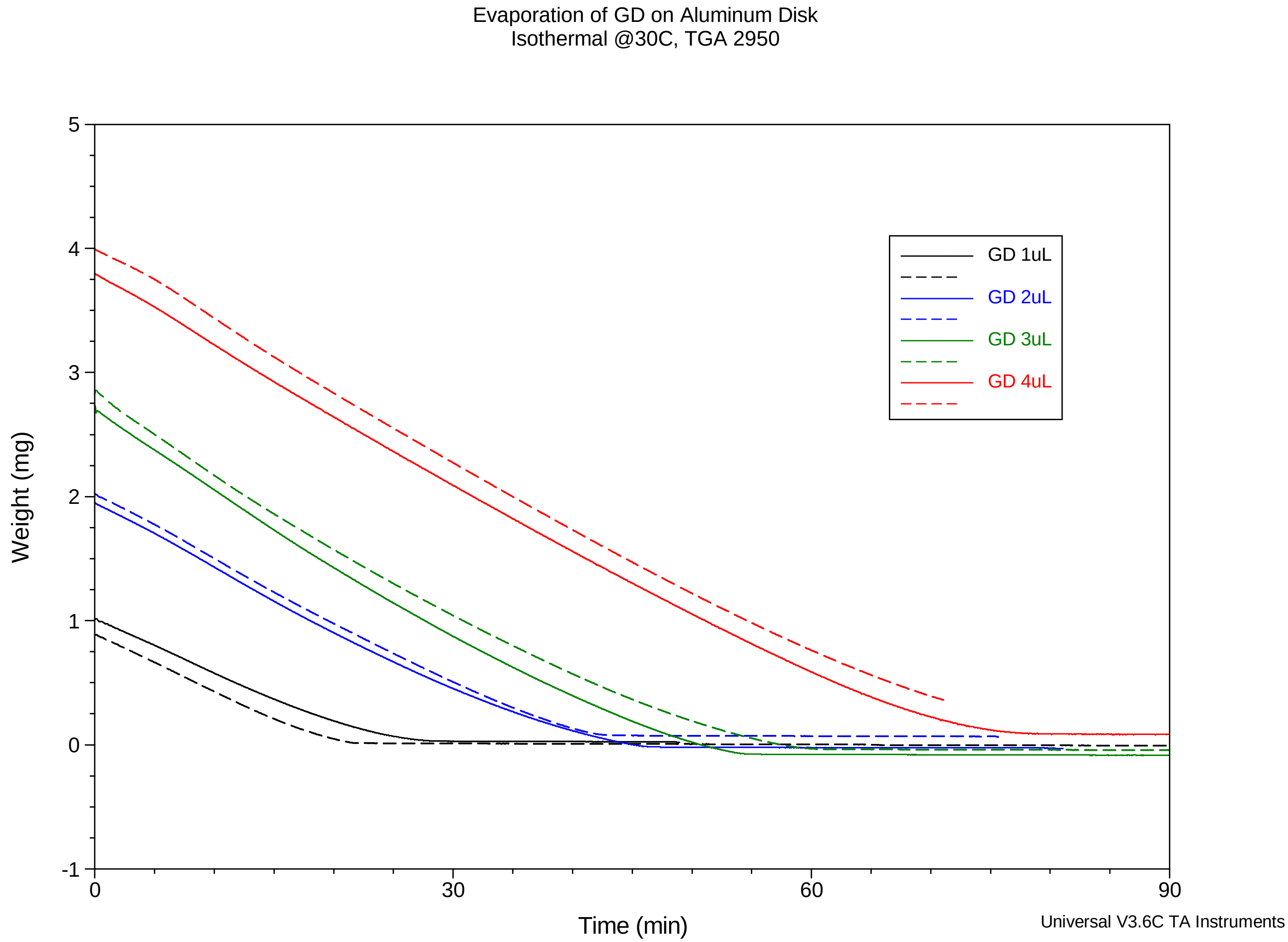


Figure. WEIGHT LOSS OF GD DROPLETS ON ALUMINUM DISKS
Isotermal @30 degrees C, Relative humidity 0%, Flow Rate 100mL/min

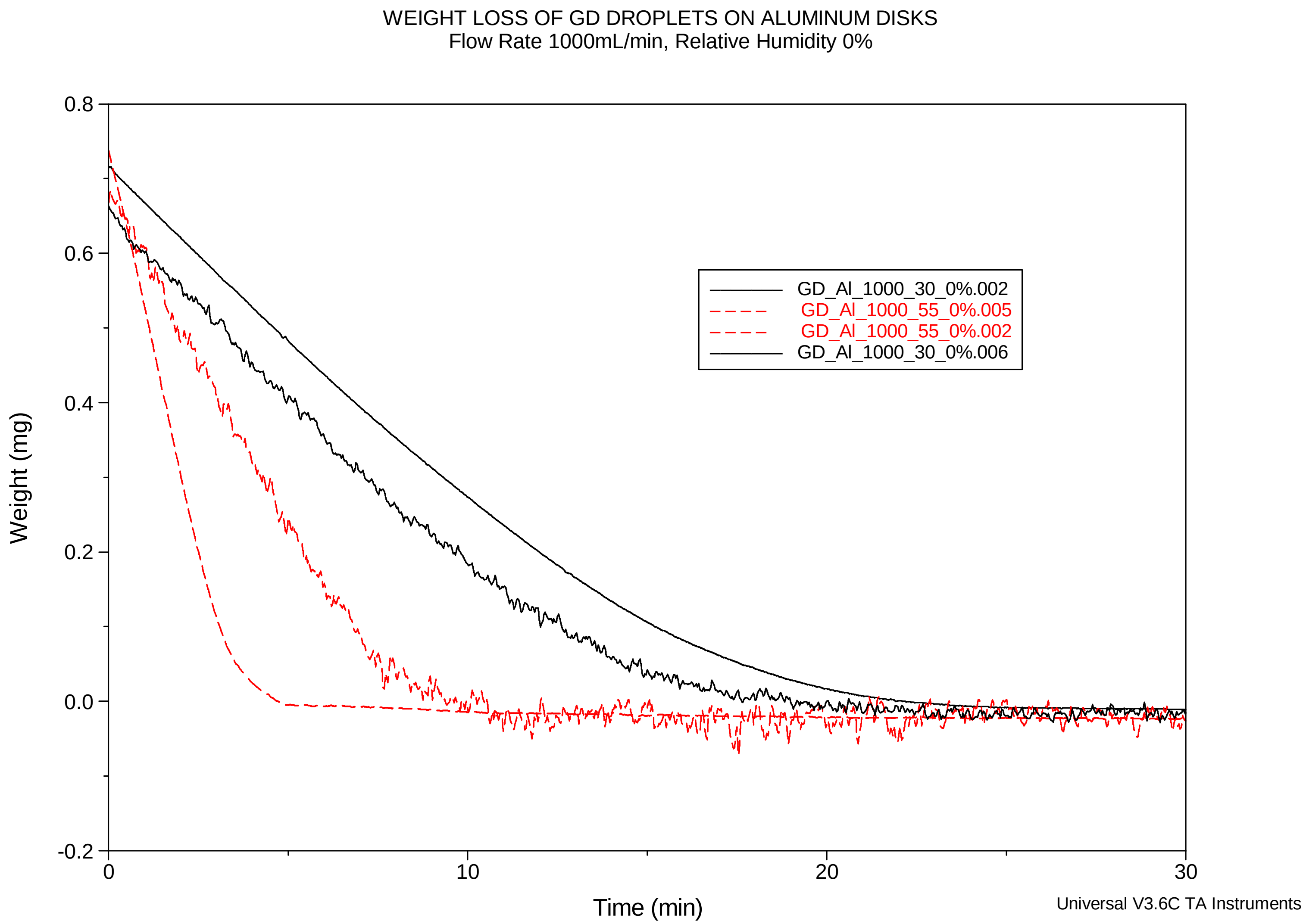


Figure. WEIGHT LOSS OF GD DROPLETS ON ALUMINUM DISKS
Relative humidity 0%, Flow Rate 1000mL/min

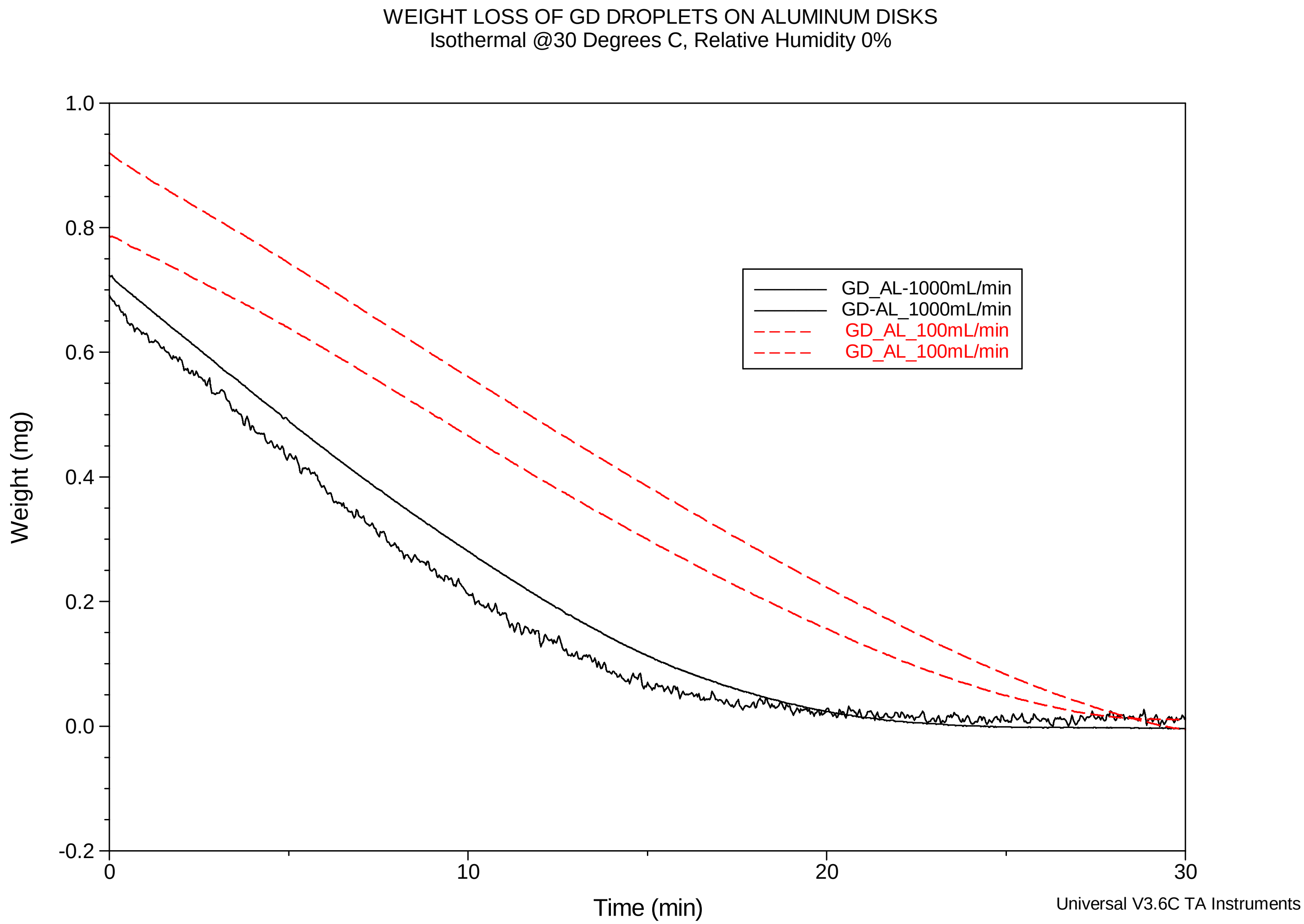


Figure. WEIGHT LOSS OF GD DROPLETS ON ALUMINUM DISKS
Isothermal @ 30 Degrees C, Relative humidity 0%

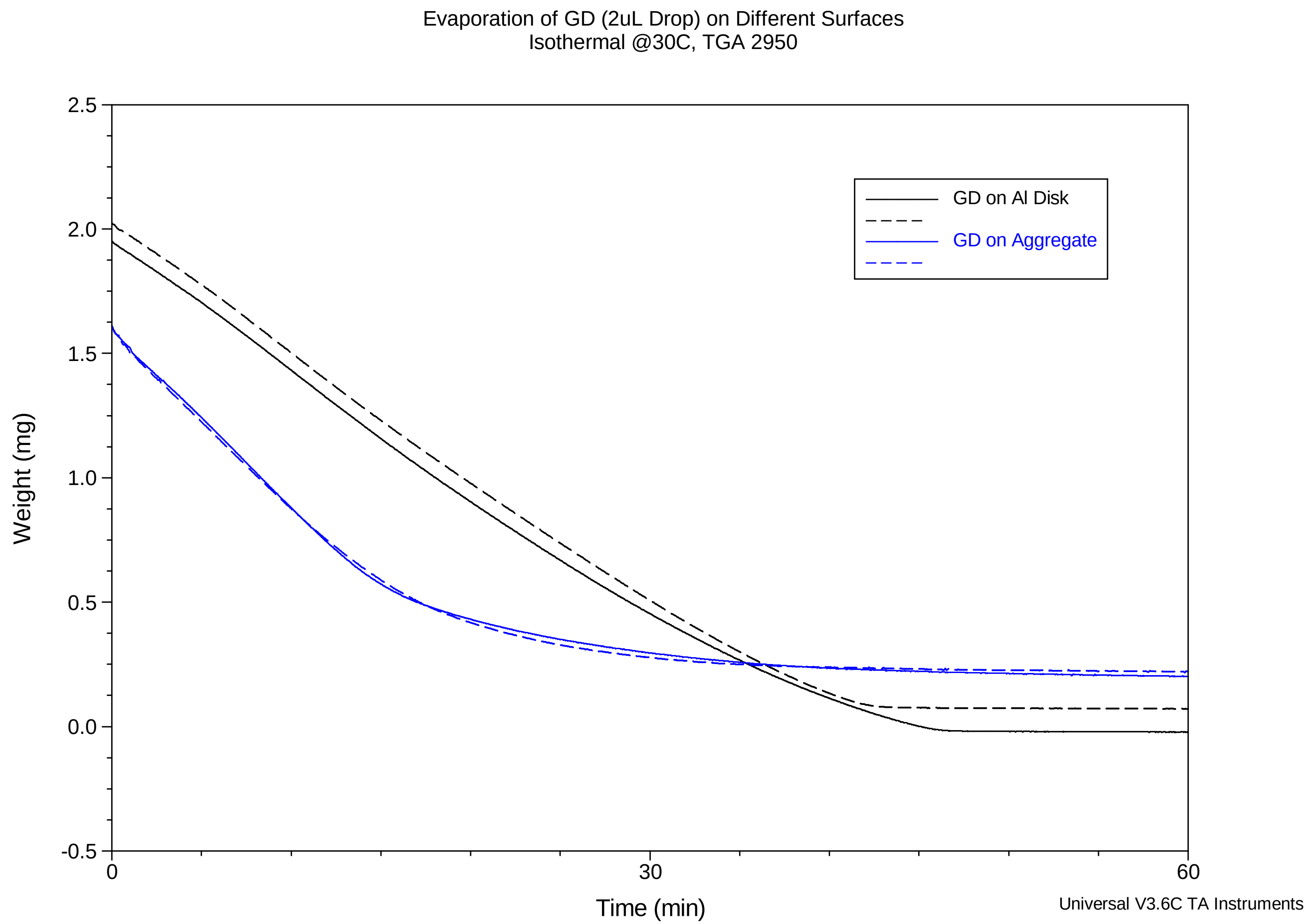
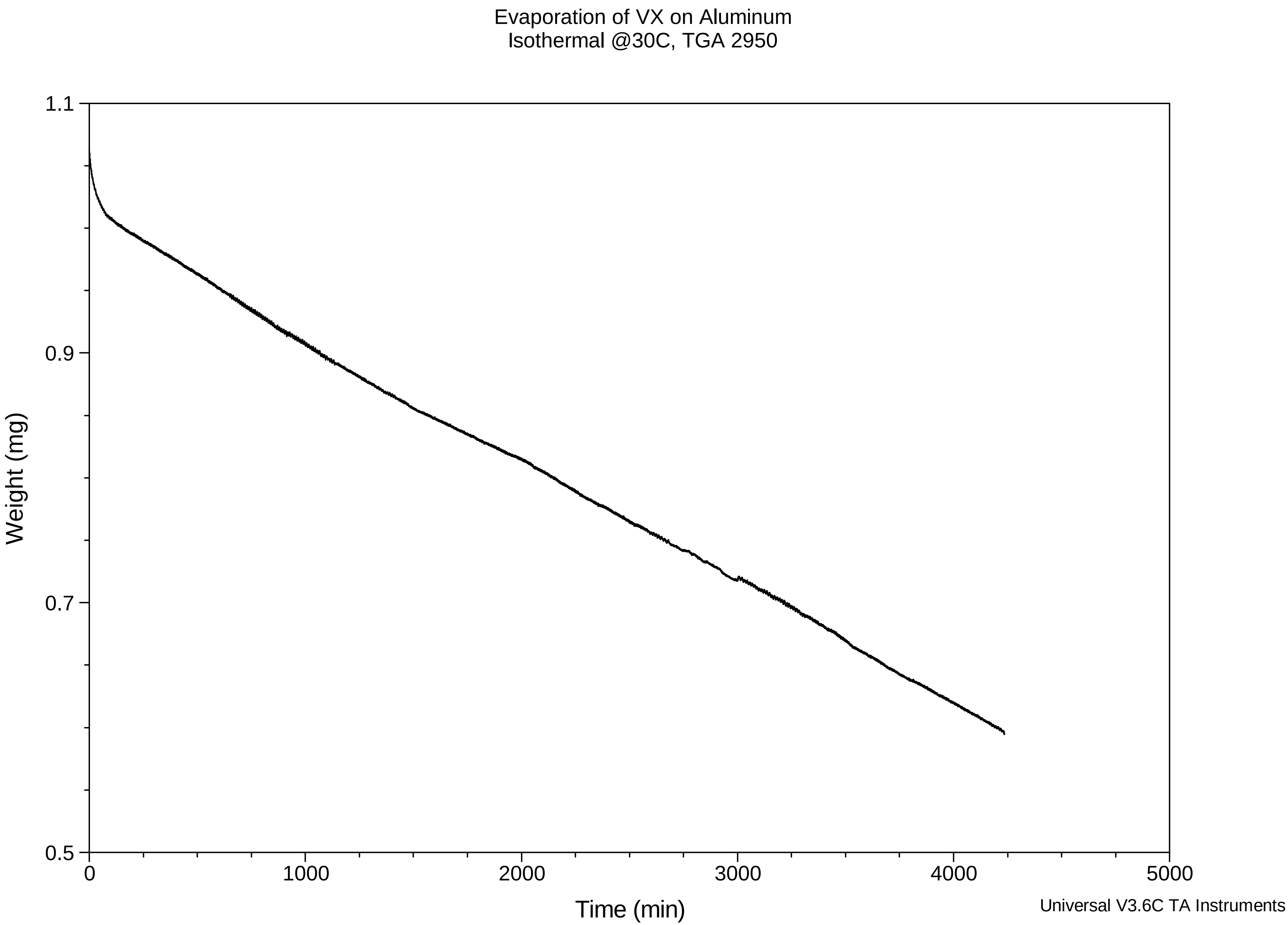


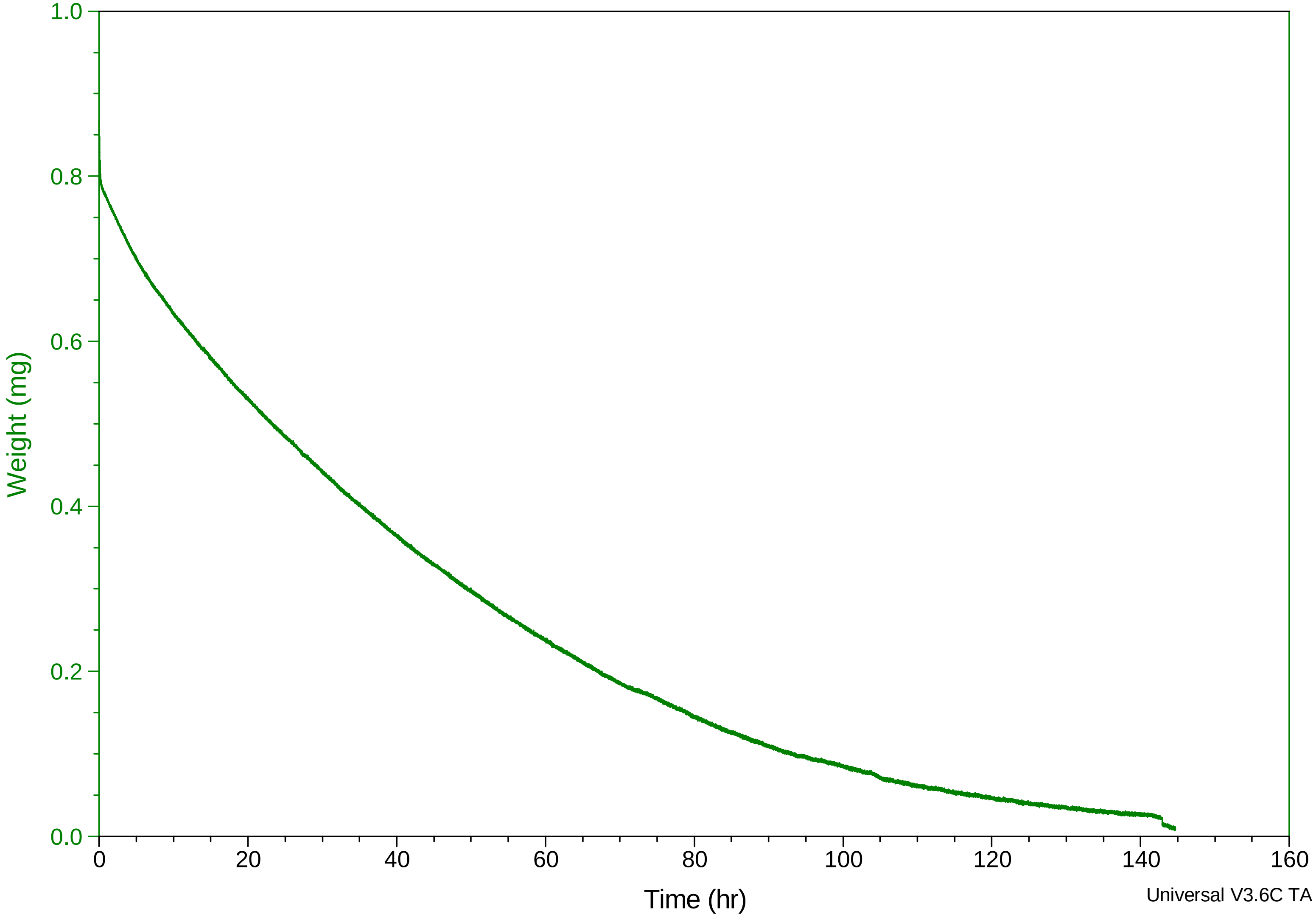
Figure. WEIGHT LOSS OF GD ON ALUMINUM DISKS vs AGGREGATE
Isothermal @ 30 Degrees C, Relative humidity 0%, Flow Rate 100mL/min


Evaporation of VX on Aluminum
Isothermal @30C, TGA 2950
Weight (mg)
1.1
0.9
0.7
0.5
0
1000
2000
3000
4000
5000
Time (min)
Universal V3.6C TA Instruments

Sample: VX-4076 ON WASHED GLASS(T) DISK
Size: 0.8660 mg
Method: KBS
Comment: VX (0.5uL) ON GLASS(T)-WASHED (6mm), @30C, 0%, 1000mL/min

DSC-TGA

File: C:...\SDT\TGA-VX\VX_GLT_30C_1000_0%.002
Operator: SHH/RGN
Run Date: 13-Aug-04 16:11
Instrument: SDT Q600 V3.9 Build 52



Universal V3.6C TA Instruments